10/565,678

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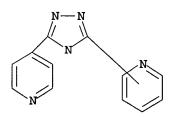
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=> d que

L1 STR



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L3 81 SEA FILE=REGISTRY SSS FUL L1

L4 53 SEA FILE=CAPLUS L3

=> d l4 1-53 ibib abs hitstr

L4 ANSWER 1 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1159571 CAPLUS

TITLE: Metabolic profile of FYX-051 (4-(5-pyridin-4-yl-1H-

[1,2,4]triazol-3-yl)pyridine-2-carbonitrile) in the

rat, dog, monkey, and human: identification of

N-glucuronides and N-glucosides

AUTHOR(S): Nakazawa, Takashi; Miyata, Kengo; Omura, Koichi;

Iwanaga, Takashi; Nagata, Osamu

CORPORATE SOURCE: Research Laboratories 2, Fuji Yakuhin Co., Ltd.,

Saitama, Japan

SOURCE: Drug Metabolism and Disposition (2006), 34(11),

1880-1886

CODEN: DMDSAI; ISSN: 0090-9556

PUBLISHER: American Society for Pharmacology and Experimental

Therapeutics

DOCUMENT TYPE: Journal

LANGUAGE: Sournat English

AB FYX-051, 4-(5-pyridin-4-yl-1H-[1,2,4]triazol-3-yl)pyridine-2-carbonitrile,

is a novel xanthine oxidoreductase inhibitor that can be used for the treatment of gout and hyperuricemia. We examined the metabolism of FYX-051 in rats, dogs, monkeys, and human volunteers after the p.o. administration of this inhibitor. The main metabolites in urine were pyridine N-oxide in rats, triazole N-glucoside in dogs, and triazole N-glucuronide in monkeys and humans, resp. Furthermore, N-glucuronidation and N-glucosidation were characterized by two types of conjugation: triazole N1- and N2-qlucuronidation and N1- and N2-glucosidation, resp. N1- and N2-qlucuronidation was observed in each species, whereas N1- and N2-glucosidation was mainly observed in dogs. With regard to the position of conjugation, N1-conjugation was predominant; this resulted in a considerably higher amount of N1-conjugate in each species than N2-conjugate. The present results indicate that the conjugation reaction observed in FYX-051 metabolism is unique, i.e., N-glucuronidation and N-glucosidation occur at the same position of the triazole ring, resulting in the generation of four different conjugates in mammals. In addition, a urinary profile of FYX-051 metabolites in monkeys and humans was relatively similar; triazole N-glucuronides were mainly excreted in urine. INDEXING IN PROGRESS

IT

577778-58-6 IT

> RL: PKT (Pharmacokinetics); BIOL (Biological study) (metabolism of antihyperuricemic drug FYX-051 in the rat, dog, monkey, and human and identification of N-glucuronides and N-glucosides)

577778-58-6 CAPLUS RN

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

22

ACCESSION NUMBER:

2006:351989 CAPLUS

DOCUMENT NUMBER:

145:54950

TITLE:

Controllable Assembly of Metal-Directed Coordination

Polymers under Diverse Conditions: A Case Study of the

MII-H3tma/Bpt Mixed-Ligand System

AUTHOR (S):

Du, Miao; Jiang, Xiu-Juan; Zhao, Xiao-Jun

CORPORATE SOURCE:

College of Chemistry and Life Science, Tianjin Normal University, Tianjin, 300074, Peop. Rep. China Inorganic Chemistry (2006), 45(10), 3998-4006

CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER:

SOURCE:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE: English

New metal-organic polymeric complexes, {[Co(bpt)(Htma)(H2O)3]·2.25H2O} n (1), [Co(bpt) (Htma) (H2O)]n (2), [Ni(bpt) (Htma) (H2O)]n (3), [Zn(bpt)2(H2tma)2]·6H2O (4), {[Cd(bpt) (Htma) (H2O)]·(EtOH) (H2O)] 0)1.5n (5), and {[Cd(bpt)(Htma)(H2O)2]·5.5H2O}n (6), were prepared from solution reactions of 4-amino-3,5-bis(4-pyridyl)-1,2,4-triazole (bpt) and trimesic acid (H3tma) with different metal salts under diverse conditions. All these compds. were structurally determined by x-ray single-crystal diffraction, and the bulk new materials were further identified by x-ray powder diffraction. Complexes 1 and 6 show 1-dimensional zigzag or linear Htma-bridged polymeric chains, with the terminal bpt ligands as pendants, which are extended to 2-dimensional

IT

CN

H-bonded arrays with 4.82 or (6,3) network topol. Coordination polymers 2 and 3, in which the 2-dimensional corrugated metal-organic frameworks make the interdigitated 3-dimensional packing, are isostructural. Complex 4 has a mononuclear structure, and its subunits are H-bonded to each other to give a 2-dimensional gridlike net. For complex 5, the CdII centers are linked by bpt/Htma ligands to form a 2-dimensional (4,4) coordination layer, and these layers are interdigitated in pairs. Notably, secondary noncovalent forces, such as H bonds, play an important role in extending and stabilizing these structural topologies. Distinct products were obtained for CoII (1 and 2) and CdII (5 and 6) under ambient or hydrothermal conditions; however, for NiII and ZnII, single products, 3 and 4, are generated. The thermal stabilities of 1-6 were studied by TGA of mass loss. The desorption/adsorption properties of the porous material 5 are also discussed. Solid-state luminescent spectra of the ZnII and CdII complexes, 4-6, indicate intense fluorescent emissions at ca. 380 nm. 38634-05-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of transition metal aminobis(pyridyl)triazole trimesic acid
coordination polymers and zinc aminobis(pyridyl)triazole trimesic acid
mononuclear complex)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)

IT 890016-34-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (polymeric; preparation, crystal structure, desorption/adsorption properties, hydrogen bonding, luminescence and thermal stability of)

RN 890016-34-9 CAPLUS

Cadmate(1-), aqua[1,3,5-benzenetricarboxylato(3-)- κ 01, κ 01'][3-(4-pyridinyl- κ N)-5-(4-pyridinyl)-4H-1,2,4-triazol-4-amine]-, (T-4)-, hydrogen, compd. with ethanol, hydrate (2:2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 890016-33-8

CMF C21 H15 Cd N6 O7 . H

CCI CCS

$$\begin{array}{c|c}
NH_2 & OH_2 \\
N & Cd & O \\
N & N-N & O
\end{array}$$

10/565,678

CM 2

CRN 64-17-5 CMF C2 H6 O

 H_3C-CH_2-OH

IT 890016-30-5P 890016-31-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (polymeric; preparation, crystal structure, hydrogen bonding and thermal stability of)

RN 890016-30-5 CAPLUS

CN Cobaltate(1-), aqua[1,3,5-benzenetricarboxylato(3-)-κ01,κ01'][3-(4-pyridinyl-κN)-5-(4-pyridinyl)-4H-1,2,4-triazol-4-amine]-, hydrogen (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
NH_2 & OH_2 \\
N & CO_2 \\
N & O \\
N & O \\
\end{array}$$

● H+

RN 890016-31-6 CAPLUS

CN Nickelate(1-), aqua[1,3,5-benzenetricarboxylato(3-)-κ01,κ01'][3-(4-pyridinyl-κN)-5-(4-pyridinyl)-4H-1,2,4-triazol-4-amine]-, hydrogen (9CI) (CA INDEX NAME)

● H+

IT 890016-35-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (polymeric; preparation, crystal structure, hydrogen bonding, luminescence and thermal stability of)

RN 890016-35-0 CAPLUS

CN Cadmate(1-), diaqua[1,3,5-benzenetricarboxylato(3-)κO1,κO1'][3-(4-pyridinyl-κN)-5-(4-pyridinyl)-4H-1,2,4triazol-4-amine]-, hydrogen, hydrate (2:11) (9CI) (CA INDEX NAME)

● H+

●11/2 H₂O

IT 890016-29-2P

> RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (polymeric; preparation, crystal structure, hydrogen bonding, pi-pi stacking interactions and thermal stability of)

RN890016-29-2 CAPLUS

CN Cobaltate (1-), triaqua [1,3,5-benzenetricarboxylato (3-)- κ 0] [3-(4pyridinyl-κN)-5-(4-pyridinyl)-4H-1,2,4-triazol-4-amine]-, hydrogen, hydrate (4:9), (SP-5-13)- (9CI) (CA INDEX NAME)

● H+

●9/4 H₂O

IT 890016-32-7P

> RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation, crystal structure, hydrogen bonding, luminescence and thermal stability of)

RN

890016-32-7 CAPLUS Zincate(4-), bis[1,3,5-benzenetricarboxylato(3-)-κ0]bis[3-(4-CN pyridinyl-κN) -5-(4-pyridinyl) -4H-1,2,4-triazol-4-amine]-, tetrahydrogen, (T-4) - (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

H+

REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2006:58796 CAPLUS

DOCUMENT NUMBER:

145:171276

TITLE:

Inhibition of mild steel corrosion in phosphoric acid

solution by triazole derivatives

AUTHOR (S):

Wang, Lin

CORPORATE SOURCE:

Department of Chemistry, Yunnan University, Yunnan,

650091, Peop. Rep. China

SOURCE:

Corrosion Science (2006), 48(3), 608-616

CODEN: CRRSAA; ISSN: 0010-938X

PUBLISHER:

Elsevier Ltd.

Journal

DOCUMENT TYPE: LANGUAGE:

English

Corrosion inhibition by triazole derivs. (n-PAT) on mild steel in phosphoric acid (H3PO4) solns. has been investigated by weight loss and polarization methods. The results indicate that these compds. act as mixed-type inhibitors retarding the anodic and cathodic corrosion reactions with emphasis on the former and do not change the mechanism of either hydrogen evolution reaction or mild steel dissoln. Some kinetic parameters are obtained.

38634-05-8 IT

RL: MOA (Modifier or additive use); USES (Uses)

(inhibition of mild steel corrosion in phosphoric acid solution by triazole derivs.)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)

THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 28 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CAPLUS COPYRIGHT 2007 ACS on STN ANSWER 4 OF 53

ACCESSION NUMBER: 2005:1305433 CAPLUS

DOCUMENT NUMBER: 144:204563

TITLE: From One- to Three-Dimensional Architectures:

Supramolecular Isomerism of Copper(I)

3,5-Di(4-pyridyl)-1,2,4-triazolate Involving in Situ

Ligand Synthesis

AUTHOR (S): Zhang, Jie-Peng; Lin, Yan-Yong; Huang, Xiao-Chun;

Chen, Xiao-Ming

CORPORATE SOURCE: State Key Laboratory of Optoelectronic Materials and

> Technologies, School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou,

510275, Peop. Rep. China

Crystal Growth & Design (2006), 6(2), 519-523 SOURCE:

CODEN: CGDEFU; ISSN: 1528-7483

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

Solvothermal treatment of Cu(II) salts, NH3, and 4-cyanopyridine was chosen for the study of supramol. isomerism of the target binary Cu(I) 3,5-di(4-pyridyl)-1,2,4-triazolate (4-pytz). A 2-dimensional coordination network of α -[Cu(4-pytz)] (1, P21/n, a 7.9633(5), b 10.3757(6), c 13.1054(8) Å, β 105.673(1)°) was obtained at 120-160° using Cu(OH)2 or Cu2(OH)2CO3 as the Cu(II) source, while a 3-dimensional network of $\beta\text{-}[\text{Cu}(4\text{-pytz})]$ (2, Cc, a 9.4278(5), b 24.7779(14), c 10.6761(6) Å, β 113.025(1)°) was obtained at 100° using Cu(OH)2 as Cu(II) source. A solvated Cu(I) 3,5-di(4-pyridyl)-1,2,4-triazolate [Cu(4-pytz)(NH3)]·4H2O (3, P21/c, a 9.2065(8), b 25.574(2), c 6.8104(6) Å, β 90.256(2)°) with 1-dimensional coordination structure also was synthesized at 100° using the Cu(NO3)2·3H2O as Cu(II) source. Novel H-bonded water-NH3 ribbons comprised of fused (H2O)5 and (H2O)4(NH3) pentagons were stabilized in the 1-dimensional channels of 3. Networks 1 and 2 show structure-related photoluminescence properties, while 3 is nonemissive under UV irritation.

IT 874895-08-6P

> RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (dimorphic; preparation and crystal structure and luminescence of polymeric)

RN874895-08-6 CAPLUS

Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis-, copper(1+) salt (9CI) CN (CA INDEX NAME)

Cu(I)

IT 874895-10-0P

> RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of polymeric)

RN 874895-10-0 CAPLUS

Copper, ammine[4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]pyridinato-CN κN]-, tetrahydrate (9CI) (CA INDEX NAME)

H20

REFERENCE COUNT:

25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4ANSWER 5 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2005:1198830 CAPLUS

DOCUMENT NUMBER:

144:99881

TITLE:

Direction of unusual mixed-ligand metal-organic

frameworks: a new type of 3-D polythreading involving

1-D and 2-D structural motifs and a 2-fold

interpenetrating porous network

AUTHOR (S):

Du, Miao; Jiang, Xiu-Juan; Zhao, Xiao-Jun

CORPORATE SOURCE:

College of Chemistry and Life Science, Tianjin Normal

University, Tianjin, 300074, Peop. Rep. China

SOURCE:

Chemical Communications (Cambridge, United Kingdom)

(2005), (44), 5521-5523

CODEN: CHCOFS; ISSN: 1359-7345

DOCUMENT TYPE:

Royal Society of Chemistry

Journal

LANGUAGE:

PUBLISHER:

English

OTHER SOURCE(S):

CASREACT 144:99881

The reaction of CuII or CdII acetate with mixed ligands terephthalic (tp) and 3,5-bis(4-pyridyl)-4-amino-1,2,4-triazole (bpt) under the same conditions affords two unusual metal-organic frameworks, in which {[Cu(tp)(bpt)(H2O)]2[Cu(bpt)2(tp)](H2O)2}n (1) represents a new type of polythreaded supramol. architecture consisting of distinct 1-dimensional and 2-dimensional coordination polymers within one crystal, whereas, ${ [Cd(tp)(bpt)(H2O)] 2 (DMF) 1.5 (H2O) }$ (2) has an interpenetrating porous network with two similar laterally interlocking 2-dimensional (4,4) layers.

IT 872411-64-8P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP

CN

(Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
 (coordination polymer; formation from thermal desorption of guest

(coordination polymer; formation from thermal desorption of guest solvates with retention of framework and re-adsorption of solvates)

RN 872411-64-8 CAPLUS

Cadmium, aqua[1,4-benzenedicarboxylato(2-)-κΟ,κΟ'][3-(4-:pyridinyl)-5-(4-pyridinyl-κN)-4H-1,2,4-triazol-4-amine]-, (T-4)-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & \text{NH}_2 \\
 & \text{N} \\
 &$$

IT 872411-65-9P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(coordination polymer; preparation and crystal structure of 2-fold interpenetrating porous network and thermal stability with desorption of solvates)

RN 872411-65-9 CAPLUS

CN Cadmium, aqua[1,4-benzenedicarboxylato(2-)-κ0][3-(4-pyridinyl-κN)-5-(-pyridinyl)-4H-1,2,4-triazol-4-amine]-, (T-4)-, compd. with N,N-dimethylformamide (4:3), dihydrate (9CI) (CA INDEX NAME)

CM 1

CRN 872411-64-8 CMF C20 H16 Cd N6 O5 CCI CCS

$$\begin{array}{c|c}
NH_2 & OH_2 \\
N & Cd & O \\
N-N & O & CO_2 - O
\end{array}$$

CM 2

CRN 68-12-2 CMF C3 H7 N O

IT 872411-63-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (coordination polymer; preparation and crystal structure of 3-D polythreading framework involving 1-D and 2-D structural motifs)

RN 872411-63-7 CAPLUS

CN Copper, aqua[1,4-benzenedicarboxylato(2-)-κ0][3-(4-pyridinyl-κN)-5-(4-pyridinyl)-4H-1,2,4-triazol-4-amine]-, compd. with [1,4-benzenedicarboxylato(2-)-κ0]bis[3-(4-pyridinyl-κN)-5-(4-pyridinyl)-4H-1,2,4-triazol-4-amine]copper (2:1), dihydrate (9CI) (CA INDEX NAME)

CM 1

CRN 872411-62-6 CMF C32 H24 Cu N12 O4 CCI CCS

$$\begin{array}{c|c}
 & CO_2^- \\
 & NH_2 \\
 & C O_2^- \\
 & NH_2 \\$$

CM 2

CRN 872411-61-5 CMF C20 H16 Cu N6 O5 CCI CCS

$$\begin{array}{c|c}
O & OH_2 \\
\hline
O & OH_2 \\
\hline
O & OH_2 \\
\hline
N & N \\
N & N \\
\hline
N & N \\
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N & N \\
N & N \\
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N & N \\
N & N \\
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N & N \\
N & N \\$$

IT 38634-05-8, 4-Amino-3,5-bis(4-pyridyl)-1,2,4-triazole
RL: RCT (Reactant); RACT (Reactant or reagent)

(for preparation of cadmium(II) and copper(II) aminobis(pyridyl)triazole terephthalate coordination polymers)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

28

ACCESSION NUMBER:

2005:971246 CAPLUS

DOCUMENT NUMBER:

143:248341

TITLE:

Synthetic pathways to a family of pyridine-containing azoles-promising ligands for coordination chemistry Nuriev, Vyatsheslav N.; Zyk, Nikolay V.; Vatsadze,

AUTHOR(S):

Sergey Z.

CORPORATE SOURCE:

Organic Chemistry Chair, Chemistry Department, M. V. Lomonosov Moscow State University, Moscow, 119992,

Russia

SOURCE:

ARKIVOC (Gainesville, FL, United States) (2005), (4),

208-224

CODEN: AGFUAR

URL: http://www.arkat-usa.org/ark/journal/2005/I04 Zef

irov/1534/1534.pdf

PUBLISHER:

Arkat USA Inc.

DOCUMENT TYPE:

Journal; (online computer file)

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 143:248341

AB A series of pyridine-containing pyrazoles, isoxazoles, imidazoles, oxazoles, thiazoles, oxadiazoles, triazoles, and 1,3,4-triazepines were synthesized as potential conjugated building blocks for the construction of coordination compds.

IT 4329-78-6P 36770-51-1P 863111-90-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of pyridyl-substituted pyrazoles, isoxazoles, imidazoles, oxazoles, thiazoles, oxadiazoles, triazoles and naphthotriazepines)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

RN 36770-51-1 CAPLUS

CN Pyridine, 3-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 863111-90-4 CAPLUS

CN Pyridine, 4,4'-[4-(4-bromophenyl)-4H-1,2,4-triazole-3,5-diyl]bis- (9CI) (CA INDEX NAME)

THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 35 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CAPLUS COPYRIGHT 2007 ACS on STN ANSWER 7 OF 53

ACCESSION NUMBER: 2005:887007 CAPLUS

DOCUMENT NUMBER:

143:399321

TITLE:

Simultaneous treatment with citrate prevents

nephropathy induced by FYX-051, a xanthine

oxidoreductase inhibitor, in rats

AUTHOR (S):

Shimo, Takeo; Ashizawa, Naoki; Matsumoto, Koji;

Nakazawa, Takashi; Nagata, Osamu

CORPORATE SOURCE:

Research Laboratories 2, Fuji Yakuhin Co., Ltd.,

Nishi-ku, Saitama, 331-0068, Japan

SOURCE:

IT

Toxicological Sciences (2005), 87(1), 267-276

CODEN: TOSCF2; ISSN: 1096-6080

PUBLISHER:

Oxford University Press

DOCUMENT TYPE:

Journal

LANGUAGE: English The possible mechanism of the underlying nephropathy found in the rat toxicity study of FYX-051, a xanthine oxidoreductase inhibitor, was investigated. Rats received oral treatment of either 1 or 3 mg/kg of

FYX-051, with and without citrate for four weeks to elucidate whether nephropathy could be caused by materials deposited in the kidney. Furthermore, anal. of the renal deposits in rats was also performed. Consequently, interstitial nephritis comprising interstitial inflammatory cell infiltration, dilatation, basophilia and epithelial necrosis of renal tubules and collecting ducts, deposits in renal tubules and collecting ducts, and so forth was seen in six of the eight rats and in all eight rats in the 1 and 3 mg/kg FYX-051 alone groups, resp., with the intensity in the 3 mg/kg group being moderate to severe. In the simultaneous treatment with citrate group, however, no alterations were observed in the kidney, except for minimal interstitial nephritis in one instance in the 3 mg/kg FYX-051 + citrate group along with an increased urinary pH, leading to an increase in xanthine solubility Anal. of intrarenal deposits showed that the entity would be composed of xanthine crystals. The present study,

therefore, showed that nephropathy in rats occurring after the

administration of FYX-051 was a secondary change caused by xanthine crystals being deposited in the kidney, and no other causes could be

577778-58-6, FYX 051

implicated in this kidney lesion.

RL: ADV (Adverse effect, including toxicity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(simultaneous treatment with citrate prevents nephropathy induced by FYX-051 in rats)

RN 577778-58-6 CAPLUS CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2005:682212 CAPLUS

DOCUMENT NUMBER:

143:156836

TITLE:

LR model of the inhibition mechanism of steel in HCl

by triazole and oxadiazole derivatives:

structure-activity correlations

AUTHOR (S):

CORPORATE SOURCE:

Bentiss, F.; Traisnel, M.; Vezin, H.; Lagrenee, M. Laboratoire de cristallochimie et physicochimie du

Solide, CNRS UPRESA 8012, ENSCL, Villeneuve d'ascq,

F-59652, Fr.

SOURCE:

International Corrosion Congress: Frontiers in Corrosion Science and Technology, 15th, Granada, Spain, Sept. 22-27, 2002 (2002), 378/1-378/8. National Centre for Metallurgical Research: Madrid,

Spain.

CODEN: 69FVP4

DOCUMENT TYPE:

Conference; (computer optical disk)

LANGUAGE: English

AB A quantum chemical study of the corrosion inhibition efficiency of triazole and oxadiazole derivs., at the mild steel electrode, in molar hydrochloric acid (1M HCl) was carried out. The correlation between the mol. structure and inhibition efficiency of these heterocyclic compds. was investigated using a linear model encompassing the charge transfer resistance (Rt). The linear resistance model (LR) was optimized with the semiempirical quant. structure activity relationships (QSAR) approach. Regression equations, with multiple correlation coeffs. superior at 0.90, were derived between 1/Rt and mol. descriptors. These significant correlations indicated that the variation of the corrosion inhibition with the structure of the inhibitors may be explained in terms of electronic properties.

IT 38634-05-8

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(linear resistance model of inhibition mechanism of steel in HCl by triazole and oxadiazole derivs. and structure-activity correlations)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:135632 CAPLUS

DOCUMENT NUMBER: 142:240433

TITLE: Preparation of 3-(2-cyanopyridin-4-yl)-1,2,4-triazoles

as xanthine oxidase inhibitors

INVENTOR(S): Nakamura, Hiroshi; Ono, Atsushi; Sato, Takahiro;

Kaneda, Shuichi

PATENT ASSIGNEE(S): Fuji Yakuhin Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

CODEN: UKAKA

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005041802	A	20050217	JP 2003-201480	20030725
PRIORITY APPLN. INFO.:			JP 2003-201480	20030725
OTHER SOURCE(S):	CASRE	ACT 142:24043	33; MARPAT 142:240433	

GI

AB The title compds. I [Rc = (un) substituted 2-cyanopyridin-4-yl; Rb = (un) substituted pyridyl, phenyl; H atom is attached to any N atom of the triazole ring], their salts, or their hydrates, useful for treatment of hyperuricemia, gout, etc., are prepared by reacting I (Rc = pyridine N-oxide-4-yl which may have substituent at any position except position 2; Rb = same as above) with cyanation agents. Thus, 1.01 g 5-(4-pyridyl-1-oxide)-3-(4-pyridyl)-1,2,4-triazole, prepared from 4-cyanopyridine N-oxide and isonicotinic hydrazide, was suspended in AcNMe2, reacted with Me3SiCN at room temperature for 10 min, and further treated

with Me2NCOCl at 60° for 6 h to give 0.79 g HCl salt of 5-(2-cyano-4-pyridyl)-3-(4-pyridyl)-1,2,4-triazole (II). The HCl salt was treated with an aqueous NaHCO3 solution in 2-butanol/H2O to give 0.60 g II. Hyperuricemic effect of II in rats was also shown.

IT 577778-58-6P, 5-(2-Cyano-4-pyridyl)-3-(4-pyridyl)-1,2,4-triazole
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN
 (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
 PREP (Preparation); USES (Uses)

(preparation of (2-cyanopyridyl)triazoles as xanthine oxidase inhibitors from (1-oxypyridyl)triazoles and cyanation agents)

RN 577778-58-6 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 837371-86-5 CAPLUS CN Pyridine, 2-methyl-4-[5-(1-oxido-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

HCl

$$Me \xrightarrow{N-N} H \xrightarrow{N} N$$

HCl

L4 ANSWER 10 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2005:99496 CAPLUS

DOCUMENT NUMBER:

INVENTOR (S):

142:198082

TITLE:

Process for preparation of 1,2,4-triazole derivatives Nakamura, Hiroshi; Uda, Junichiro; Ono, Atsushi; Sato,

Takahiro

PATENT ASSIGNEE(S):

Fujiyakuhin Co., Ltd., Japan

SOURCE:

PCT Int. Appl., 38 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND DA			ICATION		DATE .				
							20040723			
W: AE,	AG, AL,	AM, AT, A	U, AZ,	BA, BB,	BG, BR,	BW,	BY, E	BZ, CA,	CH,	
CN,	CO, CR,	CU, CZ, D	E, DK,	DM, DZ,	EC, EE,	EG,	ES, H	FI, GB,	GD,	
GE,	GH, GM,	HR, HU, I	D, IL,	IN, IS,	JP, KE,	KG,	KP, H	KR, KZ,	LC,	
LK,	LR, LS,	LT, LU, L	V, MA,	MD, MG,	MK, MN,	MW,	MX, N	IZ, NA,	NI,	
NO,	NZ, OM,	PG, PH, P	L, PT,	RO, RU,	SC, SD,	SE,	SG, S	SK, SL,	SY,	
		TR, TT, T								
		KE, LS, M								
		KZ, MD, R								
		FR, GB, G								
		BF, BJ, C	F, CG,	CI, CM,	GA, GN,	GQ,	GW, N	۱L, MR,	NE,	
	TD, TG									
AU 20042595										
CA 2531912										
EP 1650204										
		DE, DK, E					NL, S	SE, MC,	PT,	
-		RO, CY, T		• •						
JP 3779725					005-5120				723	
CN 1826335								20040	723	
US 20061898			060824		006-5656			20060		
PRIORITY APPLN.	INFO.:				003-2012					
					004-JP10	456	W	20040	723	
OTHER SOURCE(S):		MARPAT 14	2:1980	82						

This invention pertains to a method for producing 1,2,4-triazole derivs. I [wherein A = (un)substituted 1-oxopyridin-4-yl or 2-cyanopyridin-4-yl; R1 = (un)substituted pyridyl or Ph; R2 = H or a protecting group] or salts or hydrates thereof. For example, 4-cyanopyridine-N-oxide was reacted with isonicotinic acid hydrazide in MeOH in the presence of NaOMe to give 5-(1-oxopyridin-4-yl)-3-(pyridin-4-yl)-1,2,4-triazole. The triazole was reacted with benzyl chloromethyl ether in DMAc in the presence of Et3N, followed by the addition of TMSCN to afford 1-(benzyloxymethyl)-5-(2-cyanopyridin-4-yl)-3-(pyridin-4-yl)-1,2,4-triazole. The title compds. inhibit xanthine oxidase and are useful for the treatment of gout and hyperuricemia.

IT 36770-53-3P 837371-71-8P 837371-86-5P 837371-87-6P 837371-88-7P RL: IMF (Industrial manufacture); RCT

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; preparation of 1,2,4-triazole derivs.)

RN 36770-53-3 CAPLUS

CN Pyridine, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 1-oxide (9CI) (CA INDEX NAME)

RN 837371-71-8 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 577778-58-6 CMF C13 H8 N6

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 837371-86-5 CAPLUS

CN Pyridine, 2-methyl-4-[5-(1-oxido-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

RN 837371-87-6 CAPLUS CN Pyridine, 2-chloro-4-[5-(1-oxido-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

RN 837371-88-7 CAPLUS

CN Pyridine, 4-[5-(1-oxido-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-2-phenyl-(9CI) (CA INDEX NAME)

RN 577778-58-6 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 577778-84-8 CAPLUS
CN 2-Pyridinecarbonitrile, 4-[5-(2-chloro-4-pyridinyl)-1H-1,2,4-triazol-3-yl](9CI) (CA INDEX NAME)

10/565,678

RN 837371-75-2 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, hydrochloride (9CI) (CA INDEX NAME)

x HCl

RN 837371-76-3 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 577778-58-6 CMF C13 H8 N6

CM 2

CRN 7664-93-9 CMF H2 O4 S

RN 837371-77-4 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, methanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 577778-58-6 CMF C13 H8 N6

CM 2

CRN 75-75-2 CMF C H4 O3 S

RN 837371-81-0 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(2-methyl-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 577778-70-2 CMF C14 H10 N6

$$\begin{array}{c|c} & H & N \\ \hline & N & N \\ \hline & N & N \\ \end{array}$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 837371-85-4 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(2-phenyl-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 577778-85-9 CMF C19 H12 N6

$$\begin{array}{c|c} N & H & N \\ N & N & CN \end{array}$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 11 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

2004:1066921 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 142:176913

Organometallic π -tweezers incorporating pyrazine-TITLE:

and pyridine-based bridging units

AUTHOR (S): Al-Anber, M.; Stein, Th.; Vatsadze, S.; Lang, H.

CORPORATE SOURCE: Fakultaet fuer Naturwissenschaften, Lehrstuhl f.

Anorganische Chemie, Institut fuer Chemie, Technische Universitaet Chemnitz, Chemnitz, D-09111, Germany

Inorganica Chimica Acta (2005), 358(1), 50-56

SOURCE: CODEN: ICHAA3; ISSN: 0020-1693

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:176913

Pyrazine- and pyridine-based π -conjugated σ -donor mols. (LL), such as pyrazine (2a), 4,4'-bipyridine (2b), 1,2-bis(4-pyridyl)ethylene (2c), 3,5-dipyridyl-1,2,4-triazole (2d), N,N'-bis(4pyridylmethylidene)benzene-1,4-diamine (2e), 2,5bis (pyridylmethylidene) cyclopentanone (2f), 2,6-bis (4pyridylmethylidene)cyclohexanone (2g) can successfully be used to span heterobimetallic π -tweezer units [{[Ti](μ - σ , π -C.tplbond.CSiMe3)2M+ ([Ti] = (η 5-C5H4SiMe3)2Ti; M = Cu, Ag). thus accessible di-cationic species [{[Ti] $(\mu-\sigma,\pi-$ C.tplbond.CSiMe3)2 $M-LL-M{Me3SiC.tplbond.C-\mu-\sigma,\pi)2[Ti]}$ 2+ (4), which are formed via the formation of [{[Ti] $(\mu-\sigma,\pi-$ C.tplbond.CSiMe3)2}M-LL]+ (3) complexes, can be isolated in yields between 66% and 99%. However, when C5H4N-CH:CH-C6H4-CH:CH-NC5H4 (5a) and C5H4N-CH:N-C6H4-CH:CH-NC5H4 (5b), resp., are reacted with { [Ti] $(\mu-\sigma,\pi-C.tplbond.CSiMe3)$ 2} AgBF4 (1c) in a 1:1 molar ratio, then the Ag(I) ion is released from the organometallic π -tweezer 1c and coordination polymers [AgBF4·5a]n (6a) and [AgBF4.5b]n (6b) along with [Ti](C.tplbond.CSiMe3)2 (7) are formed in quant. yield.

IT 4329-78-6

> RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of titanium heterobimetal \bar{l} ic silver or copper π -tweezer complexes containing π -conjugated pyrazine or pyridine-based bridging units and their reactivity)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

IT 835604-47-2P

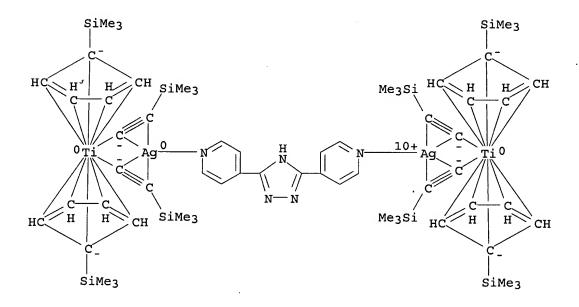
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of titanium heterobimetallic silver or copper π -tweezer complexes containing π -conjugated pyrazine or pyridine-based bridging units and their reactivity)

RN 835604-47-2 CAPLUS

CN Titanium(2+), $[[\mu-[4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[pyridine-\kappa N]]]$ disilver]tetrakis $[(1,2,3,4,5-\eta)-1-(trimethylsilyl)-2,4-cyclopentadien-1-yl]$ tetrakis $[\mu-[(1-\eta:1,2-\eta)-(trimethylsilyl)ethynyl]]$ di-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 835604-46-1 CMF C64 H97 Ag2 N5 Si8 Ti2 CCI CCS



CM 2

CRN 14797-73-0 CMF Cl O4

SOURCE:

L4 ANSWER 12 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:733660 CAPLUS

DOCUMENT NUMBER: 142:210666

TITLE: $\{ [Cu(bipy) 2.5 (H20)] (C104) 2 \cdot (H20) \cdot (CH30H) \}$

1.5}n (bipy = 4,4'-bipyridine): organic template effect in formation of a novel bilayer coordination

polymer with large chiral channels

AUTHOR(S): Du, Miao; Zhao, Xiao-Jun

CORPORATE SOURCE: College of Chemistry and Life Science, Tianjin Normal

University, Tianjin, 300074, Peop. Rep. China Inorganic Chemistry Communications (2004), 7(9),

1056-1060

CODEN: ICCOFP; ISSN: 1387-7003

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:210666

AB In the presence of the organic template mol., 4-amino-3,5-bis(4-pyridyl)-1,2,4-triazole, a unique acentric coordination polymer based on linear 4,4'-bipyridine (bipy) bridging ligand, {[Cu(bipy)2.5(H2O)](ClO4)2.

(H2O) · (MeOH) 1.5 n (1), was obtained by the reaction of Cu(II)

perchlorate with bipy in H2O/MeOH medium. The bidentate bipy mols. bridge the CuII centers to form a 2-dimensional bilayer framework with an

82.10 topol., and the monodentate bipy ligands, locating up and

down each 2-dimensional architecture, are involved in significant aromatic stacking interactions with the adjacent 2-dimensional motifs, resulting in a 3-dimensional porous network with large square channels for including the guest solvents and anions.

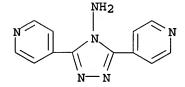
IT 38634-05-8, 4-Amino-3,5-bis(4-pyridyl)-1,2,4-triazole

RL: NUU (Other use, unclassified); USES (Uses)

(template for preparation of copper bipyridine aqua coordination polymer containing chiral channels)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:711167 CAPLUS

DOCUMENT NUMBER: 142:168214

TITLE: Synthesis and Characterization of New Coordination

Polymers Generated from Triazole-Containing Organic

Ligands and Inorganic Ag(I) Salts

AUTHOR(S): Dong, Yu-Bin; Wang, Hai-Ying; Ma, Jian-Ping; Huang,

Ru-Qi; Smith, Mark D.

CORPORATE SOURCE: College of Chemistry Chemical Engineering and

Materials Science and Shandong Key Lab of Chemical Functional Materials, Shandong Normal University,

Jinan, 250014, Peop. Rep. China

SOURCE: Crystal Growth & Design (2005), 5(2), 789-800

CODEN: CGDEFU; ISSN: 1528-7483

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal English LANGUAGE: OTHER SOURCE(S): CASREACT 142:168214 The coordination chemical of the triazole-containing rigid crooked tetradentate ligands 3,5-bis(4-pyridyl)-4-amino-1,2,4-triazole (L5) and 3,5-bis(3-pyridyl)-4-amino-1,2,4-triazole (L6) with inorg. Ag(I) salts was studied. Six new coordination polymers were prepared by solution reactions and fully characterized by IR spectroscopy, elemental anal., and single-crystal x-ray diffraction. $\{[Ag3(L5)2](NO3)3(H2O)4\}n$ (1) (triclinic, space group P.hivin.1; a 6.9481(5), b 9.7267(6), c 12.8803(8) \dot{A} , α 92.7760(10), $\dot{\beta}$ 99.1170(10), γ 104.4150(10)°, Z = 1) was obtained by the combination of L5 with AgNO3 in a H2O/MeOH mixed solvent system, and features a unique two-dimensional sheet, which consists of large tetrameric and small dimeric rings. The approx. dimensions of the rings are ca. 23 + 6 Å and 4 + 8 Å, resp. { [Ag3(L5)3](PF6)3 · (H2O) · (MeOH) n (2) (monoclinic, space group P21/n; a 10.4641(6), b 15.6701(8), c 31.1907(17) Å, β 94.8840(10)°, Z = 4) was generated from the reaction of L5 with AgPF6 in a H2O/MeOH mixed solvent system. Ag(I) centers are interlocked together by L5 through two terminal Npyridine and two Ntriazole donors into a novel noninterpenetrating three-dimensional framework with elliptical channels (effective cross-section of .apprx.12.4 + 8.0 $\mbox{\normalfont\AA}\mbox{)}$ along the crystallog. a axis. {[Ag(L5)](Cl04)·H20}n (3) (triclinic, space group P.hivin.1; a 10.3605(16), b 10.5224(16), c 15.014(2) Å, α 89.979(2), β 76.656(2), γ 89.980(2)°, Z = 4) was obtained by a combination of L5 with AgClO4 in a MeOH/H2O mixed solvent system. In the solid state, it forms a novel noninterpenetrating three-dimensional network with rhombic channels (effective cross-section of .apprx.9.0 + 8.0 Å) along the crystallog. a axis, in which noncoordinated ClO4- anions and H2O guest mols. are located. {[Ag(L6)](ClO4)·MeOH}n (4) (monoclinic, space group C2/c; a 14.1747(10), b 16.2713(11), c 15.9983(11) Å, β 114.9410(10)°, Z = 8) was obtained by the combination of L6 with AgClO4 in a MeOH/H2O mixed solvent system. In the solid state, 4 features a novel noninterpenetrating three-dimensional framework with honeycomb-like and elliptical channels in two different crystallog. directions. Their dimensions are 8 + 7 and 18 + 4 Å, resp. Uncoordinated ClO4- counterions and MeOH guest mols. are located in these channels. {[Ag(L6)](PF6)·MeOH}n (5) is generated from L6 and AgPF6 in a H2O/MeOH mixed solvent system and crystallizes in the space group C2/c, with a 15.2035(10), b 16.5919(11), c 16.1240(10) \mathring{A} , \mathring{B} $116.8490(10)^{\circ}$, Z = 8. and is isostructural with 4. ${[Ag2(C12H10N6)2](SiF6) \cdot 2H2O}n$ (6) (monoclinic, space group P21/c, a 11.3839(6), b 16.5163(8), c 7.4485(4) Å, β 95.5450(10)°, Z = 2) was obtained by the combination of L6 ligand with AgSbF6 in a MeOH/water solvent system. In the solid state, compound 6 adopts a noninterpenetrating two-dimensional net. Uncoordinated SiF62- anions and H2O mols. are located between the layers and further linked by extensive H-bonding systems into a three-dimensional framework. When viewed down the crystallog. [101] direction, honeycomb-like channels were found, in which SiF62- counterions and H2O guest mols. are located. IT 778592-76-0P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure and fluorescence spectra of noninterpenetrating three-dimensional framework with elliptical channels) RN 778592-76-0 CAPLUS CN Silver(1+), (3,5-di-4-pyridinyl-4H-1,2,4-triazol-4-amine-κN1)-, hexafluorophosphate(1-), compd. with methanol (3:1), monohydrate (9CI) (CA INDEX NAME)

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10/565,678
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CRN 67-56-1 CMF C H4 O

 H_3C-OH

CM . 2

CRN 778592-75-9 CMF C12 H10 Ag N6 . F6 P

> CM ٠3

CRN 778592-74-8 CMF C12 H10 Ag N6 CCI CCS

CM

CRN 16919-18-9 CMF F6 P CCI CCS

778592-78-2P IT

> RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of noninterpenetrating three-dimensional framework with rhombic channels)

RN

778592-78-2 CAPLUS Silver(1+), (3,5-di-4-pyridinyl-4H-1,2,4-triazol-4-amine-κN1)-, perchlorate, monohydrate (9CI) (CA INDEX NAME) CN

CM 1

778592-77-1 CRN CMF C12 H10 Ag N6 . Cl O4

> CM 2

CRN 778592-74-8 CMF C12 H10 Ag N6 CCI · CCS

CM 3

CRN 14797-73-0 CMF Cl O4

IT 38634-05-8

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant for preparation of silver(I) bis(pyridyl)aminotriazole
 coordination polymers)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:474117 CAPLUS

DOCUMENT NUMBER:

141:186841

TITLE:

The crystal structure of xanthine oxidoreductase

during catalysis: Implications for reaction mechanism

and enzyme inhibition

AUTHOR (S):

Okamoto, Ken; Matsumoto, Koji; Hille, Russ; Eger,

Bryan T.; Pai, Emil F.; Nishino, Takeshi

CORPORATE SOURCE:

Department of Biochemistry and Molecular Biology,

Nippon Medical School, Tokyo, 113-8602, Japan

SOURCE:

Proceedings of the National Academy of Sciences of the

United States of America (2004), 101(21), 7931-7936 CODEN: PNASA6; ISSN: 0027-8424

PUBLISHER:

National Academy of Sciences

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Molybdenum is widely distributed in biol. and is usually found as a mononuclear metal center in the active sites of many enzymes catalyzing oxygen atom transfer. The molybdenum hydroxylases are distinct from other biol. systems catalyzing hydroxylation reactions in that the oxygen atom incorporated into the product is derived from water rather than mol. oxygen. Here, we present the crystal structure of the key intermediate in the hydroxylation reaction of xanthine oxidoreductase with a slow substrate, in which the carbon-oxygen bond of the product is formed, yet the product remains complexed to the molybdenum. This intermediate displays a stable broad charge-transfer band at ≈640 nm. The crystal structure of the complex indicates that the catalytically labile Mo-OH oxygen has formed a bond with a carbon atom of the substrate. In addition, the Mo=S group of the oxidized enzyme has become protonated to afford Mo-SH on reduction of the molybdenum center. In contrast to previous assignments, we find this last ligand at an equatorial position in the square-pyramidal metal coordination sphere, not the apical position. A water mol. usually seen in the active site of the enzyme is absent in the present structure, which probably accounts for the stability of this intermediate toward ligand displacement by hydroxide.

IT 738626-69-2

RL: BSU (Biological study, unclassified); BIOL (Biological study) (atomic resolution crystallog. structure of xanthine oxidoreductase substrate

complex)

RN 738626-69-2 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(1,2-dihydro-2-oxo-4-pyridinyl)-1H-1,2,4triazol-3-yl]- (9CI) (CA INDEX NAME)

577778-58-6D, FYX-051, complex with xanthine oxidoreductase RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(atomic resolution crystallog. structure of xanthine oxidoreductase substrate

complex)

RN 577778-58-6 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 15 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:48216 CAPLUS

DOCUMENT NUMBER:

140:260524

TITLE:

Modulation of Heterogeneous Electron-Transfer Dynamics

PUBLISHER:

Across the Electrode/Monolayer Interface

AUTHOR (S): Walsh, Darren A.; Keyes, Tia E.; Forster, Robert J. CORPORATE SOURCE:

National Center for Sensor Research, Dublin City

University, Dublin, Ire.

SOURCE: Journal of Physical Chemistry B (2004), 108(8),

2631-2636

CODEN: JPCBFK; ISSN: 1520-6106

American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB Spontaneously adsorbed monolayers of [Os(bpy)24bptCl] (PF6) were formed on Pt microelectrodes (bpy is 2,2'-bipyridyl, and 4bpt is 3,5-bis(pyridin-4-yl)-1,2,4-triazole). These monolayers exhibit well-defined, almost ideal electrochem. responses over a wide range of voltammetric scan rates and in a wide range of electrolytic solns. Osmium bipyridine. The surface coverage of these monolayer films is consistent with that expected for a close-packed monolayer, in which the area of occupation is governed by the area of the redox-active headgroup rather than by the bridging ligand. The differential capacitance of the monolayer-modified interface is 18 \pm 3 μF cm-2 compared to 35 \pm 3 μF cm-2 for an unmodified surface. Consistent with the observation that the formal potential of the Os2+/3+ process shifts by <30 mV upon immobilization, these data suggest that the monolayers are well solvated. The dependence of the differential capacitance on solution pH reveals that the pKa of the triazole bridge within the monolayer, 8.9 ± 0.3, is indistinguishable from that found in solution Chronoamperometry, conducted on a nanosecond time scale, reveals that the redox switching mechanism involves hole rather than electron transfer. Significantly, upon protonation of the 4bpt bridging ligand, the standard heterogeneous hole transfer rate constant decreases from 1.60 to 0.2 + 106 s-1 for the reduction mechanism and from 2.7 to 0.05 + 106 s-1 for the oxidation process. These observations are consistent with the redox mechanism occurring via a hole-transfer process, the rate of which depends on the energy difference between the metal d π orbitals and the HOMO of the bridge. Protonation of the bridging ligand increases this energy gap, resulting in an overall decrease in the rate of the redox reaction. IT 671788-45-7

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(formal redox potential of adsorbed monolayer on platinum microelectrode in aqueous Na2SO4 solution)

671788-45-7 CAPLUS RN

Osmium(2+), bis(2,2'-bipyridine- κ N1, κ N1')chloro[4-[5-(4pyridinyl)-1H-1,2,4-triazol-3-yl]pyridinato-κN]- (9CI) (CA INDEX NAME)

10/565,678

IT 215366-94-2

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(spontaneously adsorbed on platinum microelectrode and modulation of heterogeneous electron-transfer dynamics across electrode/monolayer interface)

RN 215366-94-2 CAPLUS

CN Osmium(1+), bis(2,2'-bipyridine-κN1,κN1')chloro[4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]pyridine-κN]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:610439 CAPLUS

DOCUMENT NUMBER:

139:164794

TITLE:

Preparation of 1,2,4-triazole derivatives for

treatment of hyperuricemia

INVENTOR(S): Nakamura, Hiroshi; Kaneda, Soichi; Sato, Takahiro;

Ashizawa, Naoki; Matsumoto, Koji; Iwanaga, Takashi;

Inoue, Tsutomu

PATENT ASSIGNEE(S): Fuji Yakuhin Co., Ltd., Japan

SOURCE:

PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

. 1

PATENT INFORMATION:

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WO	WO 2003064410							WO 2002-JP12662						20021203				
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		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE	Ξ,]	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN	1 , 1	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
		PL,	PT,	RO,	RU,	SD,	SE,	SG,	SK,	SI	٠, ١	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,
							ZA,											
	RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ	Ζ, '	ΤZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
							TM,											
		FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NI	١, ١	PΤ,	SE,	SI,	SK,	TR,	BF,	ВJ,
		CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	MI	Ĺ, l	MR,	NE,	SN,	TD,	TG		
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BR	2002	0127	75		Α		2004	1013		CA 2002-2462132 BR 2002-12775					20021203			
EP	1471	065	065			A1 20041027			EP 2002-781876						20021203			
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							RO,											
JP	3600	832			B2		2004	1215		JP	20	03-5	640	3 3		2	0021	203
CN	3600 1561	340			Α		2005	0105		CN	200	02-8	3192	76		2	0021	203
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US	7074	816			B2		2006	0711										
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														562			0021	
OTHER S	OURCE	(S):			MARI	PAT	139:	16479	94									

$$R^3$$
 $N + N$
 R^2
 R^2

GI

AB The title compds. I [R2 represents (un) substituted pyridyl; R1 represents (un) substituted pyridyl, etc.; and R3 represents hydrogen or pivaloyloxy-substituted lower alkyl which is bonded to a nitrogen atom of the 1,2,4-triazole ring] are prepared The bioactivity of compds. of this invention was demonstrated.

IT 577778-58-6P 577778-70-2P 577778-74-6P
577778-82-6P 577778-84-8P 577778-85-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(preparation of 1,2,4-triazole derivs. for treatment of hyperuricemia) RN 577778-58-6 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 577778-70-2 CAPLUS
CN 2-Pyridinecarbonitrile, 4-[5-(2-methyl-4-pyridinyl)-1H-1,2,4-triazol-3-yl](9CI) (CA INDEX NAME)

$$\stackrel{\mathsf{Me}}{\longrightarrow} \stackrel{\mathsf{H}}{\longrightarrow} \stackrel{\mathsf{N}}{\longrightarrow} \stackrel{\mathsf{N}}{\longrightarrow} \stackrel{\mathsf{N}}{\longrightarrow} \stackrel{\mathsf{CN}}{\longrightarrow} \stackrel{\mathsf{CN}}{\longrightarrow} \stackrel{\mathsf{CN}}{\longrightarrow} \stackrel{\mathsf{CN}}{\longrightarrow} \stackrel{\mathsf{N}}{\longrightarrow} \stackrel{\mathsf{$$

RN 577778-74-6 CAPLUS

CN Pyridine, 2-chloro-4-[5-(2-methyl-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

RN 577778-82-6 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(1-oxido-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

RN 577778-84-8 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(2-chloro-4-pyridinyl)-1H-1,2,4-triazol-3-yl](9CI) (CA INDEX NAME)

RN 577778-85-9 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(2-phenyl-4-pyridinyl)-1H-1,2,4-triazol-3-yl](9CI) (CA INDEX NAME)

IT 577778-88-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 1,2,4-triazole derivs. for treatment of hyperuricemia)

RN 577778-88-2 CAPLUS

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-,
 mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 577778-58-6 CMF C13 H8 N6

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

REFERENCE COUNT:

THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2003:444294 CAPLUS

DOCUMENT NUMBER:

138:401667

TITLE:

An improved procedure for the deamination of

symmetrical 3,5-disubstituted 4-amino-1,2,4-triazoles

Bentiss, Fouad; Lagrenee, Michel; Vezin, Herve;

Bouanis, Marya; Mernari, Buchaib

CORPORATE SOURCE:

Laboratoire de Cristallochimie et Macromoleculaire,

CNRS UPRESA, Villeneuve d'Ascq, Fr.

SOURCE:

Journal of Heterocyclic Chemistry (2002), 39(1), 93-96

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER:

AUTHOR (S):

HeteroCorporation

DOCUMENT TYPE:

Journal

LANGUAGE:

English CASREACT 138:401667

OTHER SOURCE(S): CASREACT 13
AB A number of sym 3 5-disubstitu

AB A number of sym. 3,5-disubstituted 4H-1,2,4-triazole have been synthesized in good yields by deamination of the corresponding 4-amino-1,2,4-triazoles

10/565,678

via reductive diazotization of these amino compds. in the presence of hypophosphorous acid. Anal., spectral data, and theor. calcns. confirmed the structures of the new triazole derivs.

IT 38634-05-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(deamination of sym. 3,5-disubstituted 4-amino-1,2,4-triazoles by reductive diazotization in presence of hypophosphorous acid)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)

IT 4329-78-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (deamination of sym. 3,5-disubstituted 4-amino-1,2,4-triazoles by reductive diazotization in presence of hypophosphorous acid)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2003:90594 CAPLUS

DOCUMENT NUMBER:

138:385367

TITLE:

A facile and solvent-free synthesis of

3,5-disubstituted 4-amino-1,2,4-triazoles by reactions

of aromatic nitriles with hydrazine

AUTHOR (S):

Ikemi, Yukio; Hayashi, Naolo; Kakehi, Akikazu;

Matsumoto, Ktyoshi

CORPORATE SOURCE:

Graduate School of Human and Environmental Studies,

Kyoto University, Kyoto, 606-8501, Japan

SOURCE:

Heterocyclic Communications (2002), 8(5), 439-442

CODEN: HCOMEX; ISSN: 0793-0283

PUBLISHER:

Freund Publishing House Ltd.

DOCUMENT TYPE:

Journal English

LANGUAGE: OTHER SOURCE(S):

CASREACT 138:385367

GI

$$\begin{array}{c|c}
N-N \\
N \\
N \\
NH_2
\end{array}$$

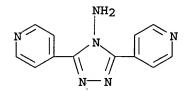
AB Triazoles I [R = 2-furanyl, 2-thienyl, indol-5-yl, 9-anthracenyl, (un)substituted phenyl] were prepared from aromatic nitriles and hydrazine monohydrate. The structure of I (R = Ph) was established by x-ray anal.

IT 38634-05-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (solvent-free synthesis of 3,5-disubstituted 4-amino-1,2,4-triazoles by reaction of aromatic nitriles with hydrazine)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:929802 CAPLUS

DOCUMENT NUMBER: 138:277681

TITLE: Redox switching in solid deposits: triazole bridged

osmium dimers

AUTHOR(S): Walsh, Darren A.; Keyes, Tia E.; Forster, Robert J.

CORPORATE SOURCE: School of Chemical Sciences, National Centre for

Sensor Research, Dublin City University, Dublin, 9,

Ire.

SOURCE: Journal of Electroanalytical Chemistry (2002),

538-539, 75-85 CODEN: JECHES

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

Solid deposits of the dimeric complex [Os(bpy)2Cl 4-bpt Os(bpy)2Cl]PF6, where bpy is 2,2'-bipyridyl and bpt is 3,5-bis(pyridin-4-yl)-1,2,4,triazole have been deposited onto platinum microelectrodes. These layers exhibit unusually ideal electrochem. responses over a wide range of electrolyte compns. and pH values. SEM reveals that repeated switching of the redox composition of these layers does not induce any significant structural change within the deposits. Cyclic voltammetry (CV) has been used to determine the apparent charge transport diffusion coefficient, DCT, describing homogeneous charge transport through the deposit. DCT is independent of the electrolyte concentration suggesting that electron self-exchange between adjacent redox centers limits the overall rate of charge transport through the solid. In 1.0 M LiClO4 and 1.0 M HClO4, DCT values of $2.0\pm0.1+10-10$ and $1.7\pm0.4+10-10$ cm2 s-1 are observed, corresponding to second order electron transfer rate consts. of 1.8+107 and 3.0+107 M-1 s-1, resp. The rate of heterogeneous electron transfer across the electrode | deposit interface has been determined using fast scan CV. The standard heterogeneous electron transfer rate constant,

k°, is 1.08±0.05 cm s-1 irresp. of the electrolyte pH.
Significantly, this value is less than one order of magnitude smaller than
that determined for a monomeric complex containing the same bridging ligand and
redox active metal center.

IT 503275-54-5P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP

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10/565,678
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(Preparation); PROC (Process) (redox switching in solid triazole bridged osmium dimers) RN 503275-54-5 · CAPLUS CN Osmium(1+), tetrakis(2,2'-bipyridine- κ N1, κ N1')dichloro[μ -[[4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[pyridinato-kN]](1-)]di-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME) CM 1 CRN 503275-53-4 CMF C52 H40 Cl2 N13 Os2 CCI CCS

CM 2 CRN 16919-18-9 CMF F6 P

CCS

CCI

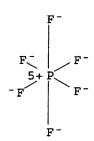
IT 215366-95-3P RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); PROC (Process); RACT (Reactant or reagent) (starting reagent in synthesis of [Os(bpy)2Cl 4-bpt Os(bpy)2Cl]PF6, where bpy is 2,2'-bipyridyl and bpt is 3,5-bis(pyridin-4-yl)-1,2,4,triazole) RN 215366-95-3 CAPLUS Osmium(1+), bis(2,2'-bipyridine- κ N1, κ N1')chloro[4-[5-(4-CNpyridinyl)-1H-1,2,4-triazol-3-yl]pyridine-κN]-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME) CM1 CRN 215366-94-2

CRN 215366-94-2 CMF C32 H25 Cl N9 Os CCI CCS

CM 2

CRN -16919-18-9

CMF F6 P



REFERENCE COUNT:

24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 20 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2002:661848 CAPLUS

DOCUMENT NUMBER:

137:331284

TITLE:

4-Amino-3,5-bis(4-pyridyl)-1,2,4-triazole

AUTHOR (S):

Guo, Ya Mei; Du, Miao

CORPORATE SOURCE:

Department of Chemistry, Tianjin University, Tianjin,

300072, Peop. Rep. China

SOURCE:

Acta Crystallographica, Section E: Structure Reports

Online (2002), E58(9), 0966-0968 CODEN: ACSEBH; ISSN: 1600-5368

URL: http://journals.iucr.org/e/issues/2002/09/00/ya61

17/index.html

PUBLISHER:

International Union of Crystallography

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE:

English

AB Crystals of the title compound are monoclinic, space group P21/c, with a 13.176(4), b 7.125(2), c 11.859(4) Å, β 105.936(6)°; Z = 4, dc = 1.478; R = 0.054, Rw(F2) = 0.180 for 1884 reflections. The two pyridine rings form dihedral angles of 35.7(2) and 16.8(2)° with the central triazole ring. The mols. exist as centrosym. related dimers

and form a three-dimensional network through intermol. N-H...N H bonds.

38634-05-8, 4-Amino-3,5-bis(4-pyridyl)-1,2,4-triazole TΤ

RL: PRP (Properties)

(crystal structure of)

38634-05-8 CAPLUS RN

4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME) CN

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4ANSWER 21 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2001:297949 CAPLUS

DOCUMENT NUMBER:

135:76833

TITLE:

Synthesis and crystal structure of

AUTHOR (S):

4-(p-methoxyphenyl)-3,5-bis(4-pyridyl)-1,2,4-triazole Zhu, Dunru; Zhu, Xiaolei; Xu, Li; Shao, Sichang; Raj,

S. Shanmuga Sundara; Fun, Hoong-Kun; You, Xiaozeng

CORPORATE SOURCE:

Coordination Chemistry Institute, the State Key

Laboratory of Coordination Chemistry, Nanjing University, Nanjing, 210093, Peop. Rep. China

SOURCE:

Journal of Chemical Crystallography (2000), 30(6),

429-432

CODEN: JCCYEV; ISSN: 1074-1542

PUBLISHER: DOCUMENT TYPE: Kluwer Academic/Plenum Publishers

Journal

LANGUAGE:

English

I

OTHER SOURCE(S):

CASREACT 135:76833

GI

AB 4-(4-Methoxyphenyl)-3,5-bis(4-pyridyl)-1,2,4-triazole (I) was synthesized, and its crystal structure was determined by X-ray diffraction methods. I crystallized in the monoclinic space group P21/n, with a = 12.5832(6) Å, b = 7.0512(5) Å, c = 18.4669(12) Å, β = 96.826(1)°, and Dcalc = 1.345 g cm-1 for Z = 4. In the structure, two pyridyl rings, Ph

ring, and triazole ring do not share a common plane. The most favored orientation of the pyridyl rings in the crystal is that their planes are inclined toward opposite directions with respect to the triazole ring.

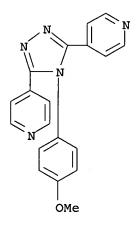
IT 346664-14-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of 4-(p-methoxyphenyl)-3,5-bis(4-pyridyl)-

1,2,4-triazole)

346664-14-0 CAPLUS RN

CN Pyridine, 4,4'-[4-(4-methoxyphenyl)-4H-1,2,4-triazole-3,5-diyl]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 22 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2001:191458 CAPLUS

DOCUMENT NUMBER:

135:98766

TITLE:

Solid deposits of osmium bis-bipyridyl triazole

chloride: Redox properties and electrocrystallization

AUTHOR (S):

Forster, Robert J.; Keyes, Tia E.

CORPORATE SOURCE:

National Centre for Sensor Research, School of Chemical Sciences, Dublin City University, Dublin,

SOURCE:

Physical Chemistry Chemical Physics (2001), 3(7),

1336-1344

CODEN: PPCPFQ; ISSN: 1463-9076

PUBLISHER:

DOCUMENT TYPE:

Royal Society of Chemistry

Journal

LANGUAGE:

English

Mech. attached, solid-state films of [Os(bpy)2(bpt)Cl] were formed on AB platinum microelectrodes and their voltammetric properties studied, bpy is 2,2'-bipyridyl and bpt is 3,5-bis(pyridin-4-yl)-1,2,4-triazole. SEM reveals that voltammetric cycling in 1.0M HClO4 converts the amorphous array of microscopically small particles into a plate-like semi-crystalline form. In contrast, crystallization does not occur when the films are cycled in 1.0M NaClO4. In both electrolytes, the voltammetric response of these films is reminiscent of that observed for an ideal reversible, solution phase redox couple. Slow and fast scan linear sweep voltammograms were used to provide an absolute determination of the fixed site concentration and apparent diffusion

coefficient, Dapp. The fixed site concentration is 1.65 \pm 0.05M for films

in either electrolyte and the Dapp values increase with increasing electrolyte concentration, Celec. These observations suggest that ion transport

rather than the rate of electron self-exchange limit the overall rate of charge transport through these solids. In 1.0M NaClO4, Dapp values for oxidation and reduction are identical at 8.3 \pm 0.5 + 10-12 cm2 s-1. In 1.0M HClO4, Dapp is significantly lower and depends on whether the deposit is being oxidized (9.7 \pm 0.4 \pm 10-13 cm2 s-1) or reduced (6.3 \pm 0.4 + 10-13 cm² s-1). These data were used to obtain an

insight into the relative importance of intra- vs. inter-particle charge transport. When Celec>0.5M, the standard heterogeneous electron transfer rate constant, k° , becomes independent of the electrolyte concentration with a value of 1.7 \pm 0.2 \pm 10-5 cm s-1 being observed in both 1.0M NaClO4 and HClO4. Significantly, the distance normalized heterogeneous electron transfer rate constant for these solid state films is almost three orders of magnitude smaller than that found within a spontaneously adsorbed monolayer of the same complex. The importance of these results for the rational design of solid-state redox active materials for battery, display and sensor applications is considered.

IT 215366-93-1

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(cyclic voltammetry of mech. attached solid-state films on platinum electrodes in HClO4 and in NaClO4 solns.: redox properties and electrocrystn.)

RN 215366-93-1 CAPLUS

CN Osmium, bis(2,2'-bipyridine-κN1,κN1')chloro[4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]pyridinato-κN]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2001:184325 CAPLUS

DOCUMENT NUMBER:

135:89700

TITLE:

N1-hetarylcarbonyl substituted amidrazone and

3,5-disubstituted 1,2,4-triazole as potential

antimycobacterial agents

AUTHOR (S):

Ranft, D.; Lehwark-Yvetot, G.; Schaper, K.-J.; Buge,

Α.

CORPORATE SOURCE:

Institut fur Pharmazeutische Chemie,

Martin-Luther-Universitat Halle-Wittenberg, Halle,

D-06120, Germany

SOURCE:

Pharmazie (2001), 56(3), 266 CODEN: PHARAT; ISSN: 0031-7144

PUBLISHER:

Govi-Verlag Pharmazeutischer Verlag

DOCUMENT TYPE:

Journal German

LANGUAGE:

N1-hetarylcarbonyl-substituted amidrazones and 3,5-dihetaryl-1,2,4-triazoles were prepared and characterized. A carbonyl spacer between N1 and the N1-hetaryl substituent led to compds. that were antimycobacterially

ineffective. Antimycobacterial effectiveness of some 3,5-dihetaryl-1,2,4-triazole derivs. was moderate.

IT 36770-50-0 348624-91-9

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(N1-hetarylcarbonyl substituted amidrazone and 3,5-disubstituted 1,2,4-triazole as potential antimycobacterial agents)

RN 36770-50-0 CAPLUS

CN Pyridine, 2-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 348624-91-9 CAPLUS

CN Pyridine, 2-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 1-oxide (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 24 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

7

ACCESSION NUMBER:

2000:291026 CAPLUS

DOCUMENT NUMBER:

132:308342

TITLE:

Preparation of pyridyl-1,2,4-triazoles as acaricides

and insecticides

INVENTOR(S):

Tisdell, Francis E.; Johnson, Peter L.; Pechacek,

James T.; Bis, Scott J.; Hedge, Vidyadhar B.;

Schoonover, Joe R., Jr.; Ripa, Perry V.; Dintenfass, Leonard P.; Gifford, James M.; Thibault, Thomas D.; Ash, Mary L.; Devries, Donald H.; Martin, Timothy P.

PATENT ASSIGNEE(S):

Dow Agrosciences Llc, USA

SOURCE:

PCT Int. Appl., 68 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT	NO.			KIN	D :	DATE		į	APPL	ICAT:	ION 1	NO.		D	ATE	
WO 200	00247	35		A1		2000	0504	1	WO 1	999-1	JS24	751		1.	9991	022
W:	ΑE,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU,
	CZ,	DE,	DK,	DM,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,
	IN,	IS,	JP,	KE,	KG,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,
	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,
	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	UZ,	VN,	YU,	ZA,	ZW,	AM,	ΑZ,	BY,
-	KG,	KZ,	MD,	RU,	TJ,	TM										
RW	: GH,	GM,	ΚE,	LS,	MW,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,

DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG EP 1123287 A1 20010816 EP 1999-955132 19991022 EP 1123287 B1 20030730 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO BR 9915534 Α 20011009 BR 1999-15534 19991022 US 6413992 В1 20020702 US 1999-425091 19991022 JP 2002528447 Т 20020903 JP 2000-578305 19991022 PT 1123287 Т 2003,1231 PT 1999-955132 19991022 ES 2200566 20040301 ES 1999-955132 19991022 PRIORITY APPLN. INFO.: US 1998-105356P 19981023 WO 1999-US24751 W 19991022 OTHER SOURCE(S): MARPAT 132:308342

AB Title compds. [I; 1 of X,Y = H, alkyl, Ph, etc. and the other = (un)substituted Ph, -pyridyl, -thienyl, etc.; Z = (un)substituted pyridyl) were prepared Thus, 3,5-dichloro-4-pyridinethioamide was S-methylated and the product N-acylated by 2,4-Cl2C6H3COCl to give ZC(SMe):NCOC6H3Cl2-2,4 (Z = 3,5-dichloro-4-pyridyl) which was cyclocondensed with MeNHNH2 to give I (X = Me, Y = C6H3Cl2-2,4, Z = 3,5-dichloro-4-pyridyl). Data for biol. activity of I were given.

CN Pyridine, 3,5-dichloro-4-[5-[6-(methylthio)-3-pyridinyl]-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

MeS C1 N N N C1

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 25 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:177112 CAPLUS

DOCUMENT NUMBER: 132:308295

DOCUMENT NUMBER

TITLE: Accelerated synthesis of 3,5-disubstituted

4-amino-1,2,4-triazoles under microwave irradiation

AUTHOR(S): Bentiss, Fouad; Lagrenee, Michel; Barbry, Didier CORPORATE SOURCE: Laboratoire de Cristallochimie et Physicochimie du

Solide, CNRS UPRESA 8012, ENSCL, Villeneuve d'Ascq,

F-59652, Fr.

SOURCE: Tetrahedron Letters (2000), 41(10), 1539-1541

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 132:308295

AB Sym. 3,5-disubstituted 4-amino-1,2,4-triazoles are quickly prepared by reaction of aromatic nitriles with hydrazine dihydrochloride in the presence of excess hydrazine hydrate in ethylene glycol under microwave irradiation

IT 38634-05-8P

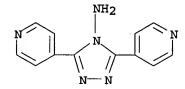
RL: SPN (Synthetic preparation); PREP (Preparation)

(accelerated synthesis of 3,5-disubstituted 4-amino-1,2,4-triazoles

under microwave irradiation)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 26 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:216715 CAPLUS

DOCUMENT NUMBER: 130:311743

TITLE: A simple one-step synthesis of new 3,5-disubstituted

4-amino-1,2,4-triazoles

AUTHOR(S): Bentiss, Fouad; Lagrenee, Michel; Traisnel, Michel;

Mernari, Bouchaib; Elattari, Hassan

CORPORATE SOURCE: Laboratoire de Cristallochimie et Physicochimie du

Solide, Ecole Nationale Superieure de Chimie de Lille

(ENSCL), Villeneuve d'Ascq, 59652, Fr.

SOURCE: Journal of Heterocyclic Chemistry (1999), 36(1),

149-152

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:311743

AB Sym. 3,5-disubstituted 4-amino-1,2,4-triazoles have been prepared by reaction of aromatic nitriles with hydrazine dihydrochloride or sulfate with an excess of hydrazine hydrate in ethylene or diethylene glycol under a

nitrogen atmospheric The structures of the new triazoles were confirmed by anal.

and spectral data.

IT 38634-05-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 27 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:644098 CAPLUS

DOCUMENT NUMBER: 129:348406

Hole superexchange across a triazole bridged osmium TITLE:

monolayer/electrode interface

AUTHOR(S): Forster, Robert J.; Vos, Johannes G.; Keyes, Tia E.

CORPORATE SOURCE: School of Chemical Sciences, Dublin City University,

Dublin, Ire.

SOURCE: Analyst (Cambridge, United Kingdom) (1998), 123(10),

1905-1911

CODEN: ANALAO; ISSN: 0003-2654

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal LANGUAGE: English

The effects of electrolyte and temperature on the electrochem. response of spontaneously adsorbed monolayers of [Os(bpy)2bptCl], where bpy is 2,2'-bipyridyl and bpt is 3,5-bis(pyridin-4-yl)-1,2,4-triazole, on clean platinum microelectrodes are reported. While cyclic voltammetry of the Os2+/3+ redox reaction is nearly ideally reversible, the bipyridyl based redns. are reversible only for scan rates .gtorsim.5 V s-1, suggesting that the highly reduced species undergoes a subsequent chemical reaction. The electrolyte concentration dependence of the double layer capacitance, Cdl, was measured for monolayers containing only Os2+ centers at potentials on either side of the potential of zero charge, p.z.c. While the limiting interfacial capacitance observed at high electrolyte concns. is .apprx.25 μF cm-2 for potentials neg. of the p.z.c., it decreases to only 12 μF cm-2 for potentials pos. of the p.z.c. Probably at pos. potentials the monolayers are relatively more perfect and contain less solvent and electrolyte ions. Oxidation of the monolayer to Os3+ causes Cdl to increase by <15%. Probably the phys. location of charges within monolayers (bridge vs. remote redox site) has a profound effect on the double layer structure. Chronoamperometry, conducted on a microsecond time-scale, was used to measure the heterogeneous electron transfer rate constant, k, for the Os2+/3+ redox reaction. For electrolyte concns. >0.1M, redox switching is characterized by a single unimol. rate constant (k/s-1). plots of the dependence of ln k on overpotential show that the rate consts. for reduction of the Os3+ centers are approx. four times larger than those for oxidation of Os2+ sites within the monolayer for a wide range of overpotentials. This observation is interpreted in terms of a bridge mediated hole superexchange mechanism. TΤ

215366-93-1

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(hole superexchange across triazole bridged osmium monolayer/electrode interface)

RN 215366-93-1 CAPLUS

Osmium, bis(2,2'-bipyridine-kN1,kN1')chloro[4-[5-(4-pyridinyl)-CN 1H-1,2,4-triazol-3-yl]pyridinato-κN]- (9CI) (CA INDEX NAME)

IT 4329-78-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with osmium bipyridine chloro complex)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

IT 215366-95-3P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(preparation: hole superexchange across triazole bridged osmium monolayer/electrode interface)

RN 215366-95-3 CAPLUS

CN Osmium(1+), bis(2,2'-bipyridine-κN1,κN1')chloro[4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]pyridine-κN]-,
hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 215366-94-2

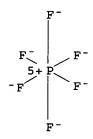
CMF C32 H25 Cl N9 Os

CCI CCS

CM 2

CRN 16919-18-9

CMF F6 P CCI CCS



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CAPLUS COPYRIGHT 2007 ACS on STN ANSWER 28 OF 53

1998:402128 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

129:70355

TITLE: Inhibiting effects of 3,5-bis(N-pyridyl)-4-amino-1,2,4-

triazoles on the corrosion for mild steel in 1 M HCl

medium

AUTHOR (S): Mernari, B.; El Attari, H.; Traisnel, M.; Bentiss, F.;

Lagrenee, M.

CORPORATE SOURCE: Laboratoire de Chimie de Coordination et d'Analytique,

Faculte des Sciences, Universite Chouaib Doukkali, El

Jadida, Morocco

SOURCE: Corrosion Science (1998), 40(2/3), 391-399

CODEN: CRRSAA; ISSN: 0010-938X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

A new class of corrosion inhibitors, namely, 3,5-bis(n-pyridyl)-4-amino-1,2,4-triazoles (n-PAT) has been synthesized and its inhibiting action on the corrosion of mild steel in 1 M HCl has been investigated by various corrosion monitoring techniques such as corrosion weight loss tests and

10/565,678

electrochem. impedance spectroscopy. The electrochem. study reveals that these compds. are anodic inhibitors. The absorption of (n-PAT) on the steel surface obeys the Langmuir adsorption isotherm.

IT 38634-05-8

RL: MOA (Modifier or additive use); PRP (Properties); USES (Uses) (inhibiting effects of 3,5-bis(N-pyridyl)-4-amino-1,2,4-triazoles on the corrosion for mild steel in 1M HCl medium)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 29 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:583321 CAPLUS

DOCUMENT NUMBER: 115:183321

TITLE: Preparation of 2-azolylnicotinates as herbicides

INVENTOR(S): Axiotis, Georges; Euvrard, Michel; Guigues, Francois;

Tadj, Fatemeh; Pearson, Christopher J.

PATENT ASSIGNEE(S): Rhone-Poulenc Agrochimie, Fr.

SOURCE: Can. Pat. Appl., 76 pp.

CODEN: CPXXEB

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

				•
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-			
CA 2027347	A1	19910421	CA 1990-2027347	19901015
FR 2653432	A1	19910426	FR 1989-14091	19891020
AU 9064699	A	19910426	AU 1990-64699	19901018
AU 629057	B2	19920924		
EP 429372	A1	19910529	EP 1990-420452	19901018
R: AT, BE, CH,	DE, DK	, ES, FR, GB	, GR, IT, LI, LU, NL,	SE
ZA 9008351	A	19910828	ZA 1990-8351	19901018
JP 03151377	Α	19910627	JP 1990-283262	19901019
CN 1051040	A	19910501	CN 1990-108601	19901020
HU 55378	A2	19910528	HU 1990-6524	19901020
BR 9005406	Α	19910917	BR 1990-5406	19901022
PRIORITY APPLN. INFO.:		•	FR 1989-14091 A	19891020
OTHER SOURCE(S):	MARPAT	115:183321		
GI	٠.			

The title compds. [I; A = H, R7SO2; R1 = H, (un)substituted (cyclo)alkyl, (hetero)aryl, aralkyl; R2 = X1M, X2R5, NR3R4, OR1; M = cation; R3, R4 = H, (un)substituted (cyclo)alkyl, aryl, aralkyl; R5 = groups cited for R1, alkenyl, alkynyl; R7 = (un)substituted (cyclo)alkyl, aryl, aralkyl, NR8R9; R8, R9 = groups cited for R1; NR8R9 = heterocyclyl; W = N, CR10; R10 = groups cited for R1; or R1R10 = atoms to form a fused ring; X1, X2 = O, S; Y = halo, alkyl, alkoxy, etc.; n = 0-3] were prepared Thus, BzNHNH2 was condensed with Et 2-cyanonicotinate to give hydrazonopyrrrolopyridine II which was refluxed 3 h with aqueous KOH to give I (A = H, R1 = Ph, R2 = OH, W = N, n = 0) which was converted in 4 steps to I (A = Me2NSO2, R1 = Ph, R2 = OH, W = N, n = 0). I.Me2CHNH2 (A = Me2SO2, R1 = 2,4-Cl2C6H3, R2 = OH, W = N, n = 0) gave complete control of 5 weeds, e.g., Echinochloa crusgalli, at 4 kg/ha preemergent.

IT 136555-59-4P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as herbicide)

RN 136555-59-4 CAPLUS

L4 ANSWER 30 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1988:112349 CAPLUS

DOCUMENT NUMBER:

108:112349

TITLE:

Studies on thio amides and their derivatives. VI. New

synthesis of 5-membered heterocyclic compounds

AUTHOR (S):

Santus, Maria

CORPORATE SOURCE:

Dep. Biochem. Gen. Chem., Acad. Med., Bydgoszcz,

85-092, Pol.

SOURCE:

Liebigs Annalen der Chemie (1988), (2), 179-82

CODEN: LACHDL; ISSN: 0170-2041

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 108:112349

GΙ

Cyclocondensation of thio amides RC(S)NHR1 (R = 2-pyridyl, R1 = 2-pyridyl, AB Ph; R = p-Me2NPh, R1 = Ph) with acid hydrazides R2CONHNH2 (I; R2 = Ph, o-HOC6H4, 4-pyridyl) in pyridine affords 29-60% triazoles II (same R-R2) via intermediate R1NHCR:NNHCOR2, which is isolated for the case R = R1 = 2-pyridyl, R2 = o-HOC6H4 from a reaction in EtOH. Cyclocondensation of I (same R2) with N,N-disubstituted thio amide quaternary salts III (R3 = H, o-HO, m-Cl, p-Br, p-O2N, p-Me2N; X = O, CH2) in pyridine affords aryloxadiazoles IV (same R2, R3).

111997-51-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

111997-51-4 CAPLUS RN

Pyridine, 2-[4-phenyl-5-(4-pyridinyl)-4H-1,2,4-triazol-3-yl]- (9CI) CN

ANSWER 31 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1977:171340 CAPLUS

DOCUMENT NUMBER:

86:171340

TITLE: AUTHOR (S): 1,2,4-Triazoles. VII. Methylation of 1,2,4-triazoles Uda, Masayuki; Hisazumi, Yukinori; Sato, Koji; Kubota,

CORPORATE SOURCE:

SOURCE:

Fac. Pharm. Sci., Univ. Tokushima, Tokushima, Japan Chemical & Pharmaceutical Bulletin (1976), 24(12),

3103 - 8

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE:

LANGUAGE:

Journal

English

Twenty-five sym. or unsym. substituted triazoles (I; R, R1 = H, Me, 2-, 3-pyridyl, MeS, Me2CH, p-R2C6H4, R2 = H, Cl, O2N) were methylated with MeI or CH2N2. The sym. substituted and monosubstituted I gave almost exclusively the 1-Me derivs. because of the α -effect of the 1,2-diaza structure or less steric hindrance, resp. However, I (R = 2-pyridyl, R1 = H) gave predominantly the 2-Me derivative due to the space effect of the pyridyl group. Methylation of 3,5-disubstituted I occurred predominantly at the N next to the electron-releasing substituent, but I (R = 2-pyridyl) were methylated mainly at the N next to the pyridyl group. IT4329-78-6 36770-50-0

RL: RCT (Reactant); RACT (Reactant or reagent) (methylation of)

RN 4329-78-6 CAPLUS CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

RN 36770-50-0 CAPLUS

CN Pyridine, 2-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 32 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:16680 CAPLUS

DOCUMENT NUMBER:

86:16680

TITLE:

1,3,5-Trisubstituted 1,2,4-triazole compounds used as

bronchodilators

INVENTOR(S):

Baldwin, John J.; Novello, Frederick C.

PATENT ASSIGNEE (S):

Merck and Co., Inc., USA

SOURCE:

U.S., 4 pp. Division of U.S. 3,882,134.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

Ι

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3984558	Α	19761005	US 1974-527994	19741129
US 3882134	A	19750506	US 1973-361914	19730521
NL 7406067	A	19741125	NL 1974-6067	19740506
SE 410458	В	19791015	SE 1974-6196	19740509
GB 1428626	A	19760317	GB 1974-21830	19740516
FR 2230357	A1	19741220	FR 1974-17249	19740517
CH 599195	A5	19780512	CH 1974-6838	19740517
JP 50025569	Α	19750318	JP 1974-59269	19740521
PRIORITY APPLN. INFO.:			US 1973-361914 A3	3 19730521
GI				

AB Triazoles I (R = CH2CH2CN, CH2CH2CO2H, CH2Ph, CH2C6H4SO2NPr2-4, CH2C6H4NO2-4, CH2C6H4Cl-3, CH2CH(OH)CH2OH, CH2C6H4Cl-4, (CH2)3OH, CH2CH2OH, CH2CH2NEt2, CH2CH2Ph, 3-picolyl, 4-picolyl, morpholinoethyl, piperidinoethyl) were prepared by substitution in I (R = H).

IT 4329-78-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkylation of)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

L4 ANSWER 33 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:577435 CAPLUS

DOCUMENT NUMBER: 85:177435

TITLE: 1,3,5-Trisubstituted 1,2,4-triazole compounds

INVENTOR(S): Baldwin, John J.; Novello, Frederick C.

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: U.S., 3 pp. Division of U.S. 3,928,361.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3978054	A	19760831	US 1975-599504	19750728
US 3882134	Α	19750506	US 1973-361914	19730521
US 3928361	Α	19751223	US 1974-527992 .	19741129
US 4048183	Α	19770913	US 1976-672899	19760402
PRIORITY APPLN. INFO.:			US 1973-361914 A	3 19730521
			US 1974-527992	3 19741129
•			US 1975-599504	3 19750728

OTHER SOURCE(S): MARPAT 85:177435

GI

AB Bronchodilatory (no data) triazoles I [R = CH2CH2CN, CH2CH2CO2H, CH2Ph, 4-Pr2NSO2C6H4CH2, 4-O2NC6H4CH2, 3-ClC6H4CH2, 3-pyridylmethyl, 4-pyridylmethyl, HOCH2CH(OH)CH2, 4-ClC6H4CH2, HO(CH2)3, HOCH2CH2, morpholinoethyl, Et2NCH2CH2, piperidinoethyl, PhCH2CH2] were prepared by substitution of I (R = H).

IT 4329-78-6

RL: RCT (Reactant); RACT (Reactant or reagent)
 (alkylation of)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

L4 ANSWER 34 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:577430 CAPLUS

DOCUMENT NUMBER: 85:177430

TITLE: Pyridyl-containing 1-benzenesulfonyl triazoles

INVENTOR(S): Novello, Frederick C.; Baldwin, John J.

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: U.S., 7 pp. Division of U.S. 3,892,762.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 3963731	A:	19760615	US 1975-547847		19750206
US 3892762	A	19750701	US 1973-361915		19730521
US 4111944	Α	19780905	US 1977-808575		19770621
PRIORITY APPLN. INFO.:			US 1970-75784	A2	19700925
			US 1973-361915	A3	19730521
			US 1975-547848	A1	19750206
			US 1976-742945	A1	19761118

GI

Uricosuric (no data) triazoles I (R = H, COPr, Me, SO2Ph, CONMe2, Pr, CH2C.tplbond.CH, allyl, Et, CHMe2, Bu; R1 = 2-methyl-4-pyridyl, 2,6-dimethyl-4-pyridyl, 2- and 3-pyridyl, 4-tolyl, 4-pyridyl N-oxide, 4-ClC6H4, Ph; R2 = pyridyl, 2-methyl-4-pyridyl, 2,6-dimethyl-4-pyridyl, , 4-pyridyl N-oxide) (30 compds.) were prepared Thus, 4-cyanopyridine was condensed with 2-methylisonicotinoylhydrazine to give I (R = H, R1 = 2-methyl-4-pyridyl, R2 = 4-pyridyl).

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

36770-45-3P 36770-46-4P 36770-47-5P

36770-48-6P 36770-50-0P 36770-53-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 36770-45-3 CAPLUS

CN Pyridine, 2-methyl-4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

$$\stackrel{N}{\underset{N-N}{\bigcup}} \stackrel{H}{\underset{||}{\underset{||}{\bigcup}}} \stackrel{N}{\underset{||}{\underset{||}{\bigcup}}}$$

RN 36770-46-4 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2-methyl- (9CI) (CA INDEX NAME)

$$\stackrel{N}{\text{Me}} \stackrel{H}{\stackrel{N}{\text{N}}} \stackrel{N}{\stackrel{N}{\text{N}}} \stackrel{N}{\stackrel{N}{\text{Me}}}$$

RN 36770-47-5 CAPLUS

Pyridine, 2,6-dimethyl-4-[5-(4-pyridinyl-1H-1,2,4-triazol-3-yl]- (9CI) CN(CA INDEX NAME)

$$\begin{array}{c|c} H \\ N \\ N \\ N \\ Me \end{array}$$

36770-48-6 CAPLUS RN

Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2,6-dimethyl- (9CI) (CA CN INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{H} & \text{Me} \\ \hline & \text{N} & \text{N} & \text{Me} \\ \hline & \text{Me} & \text{Me} \\ \end{array}$$

RN 36770-50-0 CAPLUS

CN Pyridine, 2-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

36770-53-3 CAPLUS RN

CN Pyridine, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 1-oxide (9CI) INDEX NAME)

ANSWER 35 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

84:184927

ACCESSION NUMBER: 1976:184927 CAPLUS

DOCUMENT NUMBER:

TITLE:

Antihyperuricemia composition

INVENTOR(S):

Baldwin, John J.; Novello, Frederick C.

PATENT ASSIGNEE(S):

Merck and Co., Inc., USA

SOURCE:

U.S., 7 pp. Division of U.S. 3,892,762.

CODEN: USXXAM

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3947577	Α	19760330	US 1975-539488	19750108
US 3892762	A	19750701	US 1973-361915	19730521
US 4111944	Α	19780905	US 1977-808575	19770621
PRIORITY APPLN. INFO.:			US 1970-75784 A2	19700925
			US 1973-361915 A3	19730521
			US 1975-547848 A1	19750206
			US 1976-742945 A1	19761118
OTHER SOURCE(S):	MARPAT	84:184927		

GI

3,5-Disubstituted-1,2,4-triazoles, I and II where R = H, lower alkyl, lower alkanoyl, benzenesulfonyl, carbamoyl, or lower alkylcarbamoyl, R1 = Ph, lower alkylphenyl, pyridyl, or lower alkylpyridyl, and R2 = pyridyl or lower alkylpyridyl, are useful antigout and antihyperuricemia agents. The synthesis and pharmaceutical formulations of the triazoles were described. E.g., 0.4 g Na was added to 8.3 g 4-cyanopyridine [100-48-1] in MeOH and

to this was added 0.07 mole 2-methylisonicotinic acid hydrazide
[3758-59-6] in 160 ml MeOH to give 5-(4-pyridyl)-3-(2-methyl-4-pyridyl)1,2,4-triazole [36770-45-3], m. 245-8°. Capsules containing
250 mg 3-phenyl-5-(4-pyridyl)-1,2,4-triazole [23164-60-5], 93 mg lactose,
and 7 mg talc were prepared

IT 36770-45-3 36770-47-5 36770-48-6
36770-50-0 36770-53-3
RL: BIOL (Biological study)
(antigout and antihyperuricemic agent)

RN 36770-45-3 CAPLUS
CN Pyridine, 2-methyl-4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA
INDEX NAME)

RN 36770-47-5 CAPLUS CN Pyridine, 2,6-dimethyl-4-[5-(4-pyridinyl-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-48-6 CAPLUS CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2,6-dimethyl- (9CI) (CA INDEX NAME)

RN 36770-50-0 CAPLUS CN Pyridine, 2-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-53-3 CAPLUS CN Pyridine, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 1-oxide (9CI) (CA INDEX NAME)

IT 36770-51-1

RL: BIOL (Biological study)

(in tablets, as antigout and antihyperuricemic agent)

RN 36770-51-1 CAPLUS

CN Pyridine, 3-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

IT 36770-46-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 36770-46-4 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & H & N \\ \hline N & N & M \end{array}$$

IT 4329-78-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with butyric anhydride)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

L4 ANSWER 36 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:74275 CAPLUS

DOCUMENT NUMBER: 84:74275

TITLE: 1-(Sulfamoylphenylalkyl)-3,5-dipyridyl-1,2,4 triazoles

INVENTOR(S): Baldwin, John J.; Novello, Frederick C.

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: U.S., 3 pp. Division of U.S. 3,882,134.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3928361	Α	19751223	US 1974-527992	19741129
US 3882134	Α	19750506	US 1973-361914	19730521
NL 7406067	Α	19741125	NL 1974-6067	19740506
SE 410458	В	19791015	SE 1974-6196	19740509
GB 1428626	Α	19760317	GB 1974-21830	19740516
FR 2230357	A1	19741220	FR 1974-17249	19740517
CH 599195	A5	19780512	CH 1974-6838	19740517
JP 50025569	Α	19750318	JP 1974-59269	19740521
US 3978054	Α	19760831	US 1975-599504	19750728
US 4048183	Α	19770913	US 1976-672899	19760402
PRIORITY APPLN. INFO.:			US 1973-361914	A3 19730521
			US 1974-527992	A3 19741129
			US 1975-599504	A3 19750728

GI For diagram(s), see printed CA Issue.

AB Seventeen triazoles [I; R = 3-, 4-pyridyl; R1 = NCCH2CH2, PhCH2, p-[(C3H7)2NSO2]C6H4CH2, p-O2NC6H4CH2, HO(CH2)3, 2-morpholinoethyl, etc.], useful in the treatment of asthma, the symptoms of allergy and in some instances in gout and hyperuricemia (no data), were prepared by alkylation of I (R as before; R1 = H). Thus, I (R = 4-pyridyl, R1 = H) was converted to Na salt by heating with NaH in THF and the Na salt was treated with PhCH2Cl in DMF to give I (R = 4-pyridyl, R1 = PhCH2). I (R = 4-pyridyl, R1 = NCCH2CH2) was hydrolyzed to the corresponding acid.

IT 4329-78-6

RL: RCT (Reactant); RACT (Reactant or reagent)
 (alkylation of)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

L4 ANSWER 37 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1976:59317 CAPLUS

DOCUMENT NUMBER: 84:59317

TITLE: 1,2,4-Triazol-3-ylpyridines

AUTHOR(S): Browne, Elaine J.

CORPORATE SOURCE: Dep. Chem., Univ. Tasmania, Hobart, Australia

SOURCE: Australian Journal of Chemistry (1975), 28(11), 2543-6

CODEN: AJCHAS; ISSN: 0004-9425

DOCUMENT TYPE: Journal LANGUAGE: English

AB A series of N-unsubstituted 1,2,4-triazol-3-ylpyridines was prepared for antiarthritic testing. Weak and scattered antiinflammatory activity was observed, with no clear structure-activity relationships. Some of the compds., notably the 5-pyridyl-1,2,4-triazole-3-carboxylic acids, showed infrared bands characteristic of strong H bonding.

IT 36770-50-0P 36770-51-1P 36770-53-3P 59282-64-3P 59282-65-4P 59282-66-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

10/565,678

(preparation of)

RN 36770-50-0 CAPLUS

CN Pyridine, 2-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-51-1 CAPLUS

CN Pyridine, 3-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-53-3 CAPLUS

CN Pyridine, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 1-oxide (9CI) (CA INDEX NAME)

RN 59282-64-3 CAPLUS

CN Pyridine, 3-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 1-oxide (9CI) (CA INDEX NAME)

RN 59282-65-4 CAPLUS

CN Pyridine, 3-[5-(1-oxido-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 1-oxide (9CI) (CA INDEX NAME)

RN 59282-66-5 CAPLUS

Pyridine, 2-[5-(1-oxido-4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA CN INDEX NAME)

ANSWER 38 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1976:29998 CAPLUS

DOCUMENT NUMBER:

84:29998

TITLE:

1,2,4-Triazoles. V. Nuclear magnetic resonance study

of N-methyl derivatives of 1,2,4-triazoles

AUTHOR (S):

Kubota, Seiju; Uda, Masayuki; Nakagawa, Toshiro Fac. Pharm. Sci., Univ. Tokushima, Tokushima, Japan

CORPORATE SOURCE:

SOURCE:

Journal of Heterocyclic Chemistry (1975), 12(5),

855-60

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE:

Journal English

LANGUAGE:

The chemical shifts of the N-methyl protons of a number of N-methylated-1,2,4triazoles were studied. Substitution of methyl and methylthio groups in position 3 causes upfield shifts of the N-methyl signals, while substitution of α -pyridyl, γ -pyridyl, and phenyl groups causes downfield shifts. In 3,5-disubstituted 1,2,4-triazoles, substituents in positions 3 and 5 have additive effects on the chemical shifts of N-methyl groups, so that the chemical shifts of the N-methyl groups of such compds. can be calculated In this way, it was possible to assign the peaks of mixts. of N-monomethylated derivs. obtained by methylation of 1,2,4-triazoles.

IT 4329-78-6 36770-50-0

RL: PRP (Properties)

(NMR of)

RN4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

RN 36770-50-0 CAPLUS

CN Pyridine, 2-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 39 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1975:588199 CAPLUS

DOCUMENT NUMBER: 83:188199

TITLE: 4-Trifluoromethylimidazoles and 5-(4-pyridyl)-1,2,4-

triazoles, new classes of xanthine oxidase inhibitors

AUTHOR(S): Baldwin, J. J.; Kasinger, P. A.; Novello, F. C.;

Sprague, J. M.; Duggan, D. E.

CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., West Point, PA, USA

SOURCE: Journal of Medicinal Chemistry (1975), 18(9), 895-900

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Of about 20 title imidazoles (I; R = aryl, heterocyclic, alkyl), prepared from the condensation of an aldehyde with trifluoroglyoxal in the presence of NH3, and about 16 triazoles (II), prepared by several methods, the compds. with a free imino group had xanthine oxidase [9002-17-9] inhibitory activity. 3,5-Di-4-pyridyl-1,2,4-triazole (II, R = 4-pyridyl)(III) [4329-78-6] was among the most active with an inhibition value (I50) of 6 + 10-8M, but the corresponding 1-methyl derivative of III [56932-27-5] was inactive.

IT 4329-78-6P 36770-50-0P 36770-51-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and xanthine oxidase inhibition by)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

RN 36770-50-0 CAPLUS

CN Pyridine, 2-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-51-1 CAPLUS

CN Pyridine, 3-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 40 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1975:564184 CAPLUS

DOCUMENT NUMBER: 83:164184

TITLE: 3,5-Dipyridyl-1,2,4-triazoles

INVENTOR(S): Baldwin, John J.; Novello, Frederick C.

PATENT ASSIGNEE(S): Merck and Co., Inc. SOURCE: Ger. Offen., 10 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
				-	
DE 2424404	A1	19741212	DE 1974-2424404		19740520
US 3882134	Α	19750506	US 1973-361914		19730521
NL 7406067	Α	19741125.	NL 1974-6067		19740506
SE 410458	В	19791015	SE 1974-6196		19740509
GB 1428626	A	19760317	GB 1974-21830		19740516
FR 2230357	A1	19741220	FR 1974-17249		19740517
CH 599195	A5	19780512	CH 1974-6838		19740517
JP 50025569	A	19750318	JP 1974-59269		19740521
PRIORITY APPLN. INFO.:			US 1973-361914	Α	19730521

GI For diagram(s), see printed CA Issue.

AB Seventeen triazoles I [R = e.g. CH2CH2CN, CH2CH2OH, (CH2)3OH, CH2CH2Ph, CH2C6H4SO2NPr2-4, CH2C6H4Cl-3 or -4, 3- or 4-pyridylmethyl, morpholinoethyl, or piperidinoethyl; R1 = 3- or 4-pyridyl], useful as bronchodilators (no data), were prepared by reaction of I (R = H) with ClR, BrR, or CH2:CHCN. Thus, I (R = H, R1 = 4-pyridyl) (II) and CH2:CHCN were refluxed in pyridine containing PhCH2N+Me3 OH- to give I (R = CH2CH2CN, R1 = 4-pyridyl). Successive treatment of II with NaH in THF and with PhCH2Cl in DMF at reflux gave I (R = CH2Ph, R1 = 4-pyridyl).

IT 4329-78-6 36770-51-1

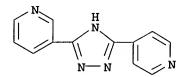
RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with organic halides)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME).

RN 36770-51-1 CAPLUS

CN Pyridine, 3-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)



L4 ANSWER 41 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1975:558007 CAPLUS

DOCUMENT NUMBER: 83:158007

TITLE: 3,5-Disubstituted 1,2,4-triazoles, a new class of

xanthine oxidase inhibitor

AUTHOR(S): Duggan, D. E.; Noll, R. M.; Baer, J. E.; Novello, F.

C.; Baldwin, J. J.

CORPORATE SOURCE: Merck Inst. Therm. Res., West. Point, PA, USA

SOURCE: Journal of Medicinal Chemistry (1975), 18(9), 900-5

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB 3,5-Bis(4-pyridyl)-1,2,4-triazole(I), 3-(4-pyrimidinyl)-5-(4-pyridyl)-1,2,4-triazole(II), and 3-(4-pyridazinyl)-5-(4-pyridyl)-1,2,4-triazole

(III) are active competitive inhibitors of xanthine oxidase, with inhibition consts. <1 + 10-7M. ED50 values in squirrel monkeys,

derived from first-order rate consts. for the first and rate-limiting step of the xanthine-uric acid-allantoin sequence, ranged from 0.04-0.08 mg/kg, orally. Sensitivity of rats, dogs, and anthrapoid species to I, II, and III is at least an order of magnitude greater than to purine analogs tested.

IT 4329-78-6

RL: BIOL (Biological study)

(xanthine oxidase inhibition by)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

L4 ANSWER 42 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1972:552130 CAPLUS

DOCUMENT NUMBER: 77:152130

TITLE: Symmetrically and unsymmetrically 3,6-disubstituted

1,2-dihydro-1,2,4,5-tetrazines including their conversion into the corresponding tetrazines and

3,5-disubstituted 4-amino-1,2,4-triazoles

AUTHOR(S): Bowie, R. A.; Gardner, M. D.; Neilson, D. G.; Watson,

K. M.; Mahmood, S.; Ridd, V.

CORPORATE SOURCE: Pharm. Div., Imp. Chem. Ind. Ltd., Macclesfield, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions

1: Organic and Bio-Organic Chemistry (1972-1999)

(1972), (19), 2395-9

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal LANGUAGE: English

AB 3,6-Disubstituted 1,2-dihydro-1,2,4,5-tetrazines were prepared by the action

IT 36770-45-3P 36770-46-4P 36770-47-5P

36770-48-6P 36770-50-0P 36770-51-1P

36770-53-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 36770-45-3 CAPLUS

CN Pyridine, 2-methyl-4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-46-4 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & H & N \\ \hline N & N & Me \end{array}$$

RN 36770-47-5 CAPLUS

CN Pyridine, 2,6-dimethyl-4-[5-(4-pyridinyl-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H \\ N \\ N \\ N \\ \end{array}$$

RN 36770-48-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2,6-dimethyl- (9CI) (CA INDEX NAME)

RN 36770-50-0 CAPLUS

CN Pyridine, 2-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

10/565,678

of H2NNH2.H2O on nitriles in the presence of S or on amidinium chlorides; the dihydrotetrazines were oxidized to the corresponding tetrazines and rearranged by heat or acid to 3,5-disubstituted 4-amino-1,2,4-triazoles. 1,2-Dihydro-1,2,4,5-tetrazines and 4-amino-1,2,4-triazoles were distinguished by PMR spectroscopy.

IT 38634-05-8

RL: PRP (Properties)

(NMR of)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)

L4 ANSWER 43 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1972:405487 CAPLUS

DOCUMENT NUMBER:

77:5487

TITLE:

5-Pyridyl-1,2,4-triazoles

INVENTOR(S):

Baldwin, John J.; Novello, Frederick C.

PATENT ASSIGNEE(S):

Merck and Co., Inc.

SOURCE:

Ger. Offen., 23 pp.

CODEN: GWXXBX

DOCUMENT TYPE:

Patent German

LANGUAGE:

- 2

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2147882	Α	19720330	DE 1971-2147882		19710924
NL 7112372	Α	19720328	NL 1971-12372		19710908
AU 7133426	Α	19730322	AU 1971-33426		19710914
CA 983504	A1	19760210	CA 1971-122846		19710914
GB 1352257	. A	19740508	GB 1971-43755		19710920
CH 564009	A5	19750715	CH 1971-13845		19710922
FR 2107985	A5	19720512	FR 1971-34443		19710924
FR 2107985	B1	19750207			
JP 50024315	В	19750814	JP 1971-74222		19710925
BE 781056	A1	19720922	BE 1972-115407		19720322
US 4111944	A	19780905	US 1977-808575		19770621
PRIORITY APPLN. INFO.:			US 1970-75784	Α	19700925
			US 1973-361915	A1	19730521
			US 1975-547848	A1	19750206
			US 1976-742945	A1	19761118

GI For diagram(s), see printed CA Issue.

AB Fourteen title compds. (I, e.g. R = 2-methyl-4-pyridyl, 2-pyridyl, 3-pyridyl, or p-MeC6H4; R1 = H, PrCO, Me, Me2NCO, or PhSO2; R2 = 4-pyridyl, 2,6-dimethyl-4-pyridyl, 3-pyridyl, or 4-pyridyl-1-oxide) useful as drugs against hyperuricemia, gout, or hypertension were prepared by reaction of R1NHNHCOR with MeOC(:NH)R2, prepared from MeOH, Na, and R2CN, and optionally if R1 = H reaction with R1Cl (R1 = PhSO2 or Me2NCO) or (PrCO)2O. Compns. for I-containing tablets and capsules are reported. Thus, Na was added to 4-cyanopyridine and MeOH. After 30 min 2-methylisonicotinoyl hydrazide was added and the mixture refluxed 30 min and heated 15 min at 260° to give I (R = 2-methyl-4-pyridyl, R1 = H, R2 = 4-pyridyl).

RN 36770-51-1 CAPLUS

CN Pyridine, 3-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-53-3 CAPLUS

CN Pyridine, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 1-oxide (9CI) (CA INDEX NAME)

L4 ANSWER 44 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1969:114407 CAPLUS

DOCUMENT NUMBER:

70:114407

TITLE:

Triazoles. X. Hydrogen bonding and infrared spectra

AUTHOR (S):

Browne, E. J.; Polya, J. B.

CORPORATE SOURCE:

Univ. Tasmania, Hobart, Australia

SOURCE:

Journal of the Chemical Society [Section] C: Organic

(1969), (7), 1056-60

CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE:

Journal English

LANGUAGE:

English

AB Ir spectra of N-unsubstituted 1,2,4-triazoles in the 1700-3000 cm.-1 region were studied, and classified according to the intensity and number of bands characteristic of strong intermol. H bonding. Evidence of groups showing different degrees of proton tunnelling is advanced; one of these groups appears to be involved in phosphorescent effects.

IT 4329-78-6

RL: PRP (Properties)

(hydrogen bonding in)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

L4 ANSWER 45 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1968:114391 CAPLUS

DOCUMENT NUMBER: 68:114391

TITLE: By-products during isolation of isonicotinic acid

hydrazide

AUTHOR(S): Basu, Uma P.; Dutta, Sakti P.

CORPORATE SOURCE: Bengal Immunity Res. Inst., Bengal, India

SOURCE: Industrie Chimique Belge (1967), 32(11), 1224-6

CODEN: ICBEAJ; ISSN: 0019-9052

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

Diisonicotinoyl hydrazine (I), hydrazodicarboxamide (II), and 3,5-di(4-pyridyl)-1,2,4-triazole-1-carboxhydrazide (III) were isolated as by-products in the large-scale production of isonicotinic acid hydrazide. They were separated from the reaction product by their varying solubilities in different solvents. I, m. 262-4°, and II, m. 244-6° (decomposition), were identified by their mixed m.p. III, m. 338-40° (decomposition), slowly reduces iodine, gives off pyridine on fusion with Na2CO3, is resistant to hydrolysis and to PCl5 or POCl3. Its hydrochloride forms a Cu complex. It is oxidized to the amphoteric 3,5-bis(4-pyridyl)-1,2,4-triazole (IV), m. 280-2°. IV was synthesized by treating isonicotinic acid hydrazide with N2H4 and CO2 or with isonicotinamide. A mechanism via H2NNHCO2H is suggested and confirmed by treating isonicotinic acid hydrazide containing H2NNHOH and CO2 with nicotinamide. A compound 3-(3-pyridyl)-5-(4-pyridyl)-1,2,4-triazole-1-carboxhydrazide, very similar to III, is obtained.

IT 4329-78-6P 18603-36-6P 36770-51-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

RN 18603-36-6 CAPLUS

CN Pyridine, 3,4'-s-triazole-3,5-diyldi-, nitrate (8CI) (CA INDEX NAME)

CM 1

CRN 36770-51-1 CMF C12 H9 N5

CM 2

CRN 7697-37-2

CMF H N O3

36770-51-1 CAPLUS RN

Pyridine, 3-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) CN(CA INDEX

ANSWER 46 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:4035 CAPLUS

64:4035 DOCUMENT NUMBER:

ORIGINAL REFERENCE NO.: 64:687g-h,688a-b

TITLE: N-Oxides and related compounds. XXVI. Ring-opening of

N-methoxypyridinium perchlorate by hydroxide ion

AUTHOR (S): Eisenthal, R.; Katritzky, A. R.

CORPORATE SOURCE: Univ. East Anglia, Norwich, UK SOURCE: Tetrahedron (1965), 21(9), 2205-13

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE:

Journal LANGUAGE: English

For diagram(s), see printed CA Issue.

cf. CA 62, 1648a. Treatment of 0.55 mole pyridine N-oxide with 0.55 mole Me2SO4 and the methosulfate in 85 ml. absolute alc. treated with 55 ml. 70% HClO4 and 400 ml. EtOAc gave 88.7 g. N-methoxypyridinium perchlorate (I), m. 69-70° (95% alc.). The time dependence of spectra of 0.10N to 1.0N I in MeONa-MeOH showed no absorbance above 275 m $\!\mu$ and rapid change of the spectrum to that of C5H5N. The kinetics of this reaction were studied by the method of initial rates. I (0.01 mole) and 0.08 mole PhNH2.HCl in 40 ml. H2O stirred at 0° with addition of 24 g. NaOH (50%

aqueous solution) and the deep red mixture made strongly acidic with 40 ml.

concentrated

HCl, the gummy product (1.2 g.) extracted with warm Me2CO and the filtered solution cooled gave 150 mg. carmine crystals of PhN: CHCH:CHCH2CH: NPh.2HCl salt, m. 168°. The available evidence was rationalized as a 1st irreversible step producing C5H5N and HCHO. In the accompanying 2nd step OH ions react rapidly but reversibly to give the 1,2-dihydropyridine derivative (II). Glutaconic aldehyde reacts with H2NOMe at pH 4.75 to yield III but examination of the product mixture at pH 9 reveals that further

reaction

proceeds rapidly from II to N-methoxypyridium ion. Accordingly at pH 4.7 the reversal of steps 2 and 3 is rapid compared with the forward reactive step 4 as shown by the observation that acidification of alkaline solns. of I results in loss of the 343 mu absorption and regeneration of the spectrum of I.

4329-78-6P, Pyridine, 4,4'-s-triazole-3,5-diyldi-TT

4334-22-9P, Pyridine, 4,4'-s-triazole-3,5-diyldi-, dipicrate

4334-23-0P, Pyridine, 4,4'-s-triazole-3,5-diyldi-, dihydrochloride

4334-24-1P, Pyridine, 4,4'-s-triazole-3,5-diyldi-, dinitrate

RL: PREP (Preparation)

(preparation of)

10/565,678

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

RN 4334-22-9 CAPLUS

CN Pyridine, 4,4'-s-triazole-3,5-diyldi-, dipicrate (7CI, 8CI) (CA INDEX NAME)

CM 1

CRN 4329-78-6 CMF C12 H9 N5

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

RN 4334-23-0 CAPLUS

CN Pyridine, 4,4'-s-triazole-3,5-diyldi-, dihydrochloride (8CI) (CA INDEX NAME)

•2 HCl

RN 4334-24-1 CAPLUS

CN Pyridine, 4,4'-s-triazole-3,5-diyldi-, dinitrate (8CI) (CA INDEX NAME)

CM 1

CRN 7697-37-2 CMF H N O3

2 CM

CRN 4329-78-6 C12 H9 N5 CMF

ANSWER 47 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

1966:4034 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 64:4034 ORIGINAL REFERENCE NO.: 64:687e-g

Abnormal products during isolation of isonicotinic TITLE:

acid hydrazide

AUTHOR (S): Basu, Uma Prasanna; Dutta, Saktipada Bengal Immunity Res. Inst., Calcutta CORPORATE SOURCE:

Journal of Organic Chemistry (1964), 30(10), 3562-4 SOURCE:

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English

For diagram(s), see printed CA Issue.

Et isonicotinate and N2H4.H2O not only afforded isonicotinic acid AB hydrazide but also symm. diisonicotinyl hydrazine (I), hydrazodicarbonamide (II), and 3,5-di(4-pyridyl)-1,2,4-triazole-1carboxhydrazide (III) in small amts. I, II, and III were separated and purified. Their structures were further confirmed by chemical reactions. Oxidation of III gave 3,5-di(4-pyridyl)-1,2,4-triazole. The mechanism of the

reaction was discussed. IT 4329-78-6P, Pyridine, 4,4'-s-triazole-3,5-diyldi-

4334-22-9P, Pyridine, 4,4'-s-triazole-3,5-diyldi-, dipicrate
4334-23-0P, Pyridine, 4,4'-s-triazole-3,5-diyldi-, dihydrochloride
4334-24-1P, Pyridine, 4,4'-s-triazole-3,5-diyldi-, dinitrate

RL: PREP (Preparation)

(preparation of) 4329-78-6 CAPLUS

Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME) CN

RN

10/565,678

CN Pyridine, 4,4'-s-triazole-3,5-diyldi-, dipicrate (7CI, 8CI) (CA INDEX NAME)

CM 1

CRN 4329-78-6 CMF C12 H9 N5

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

$$O_2N$$
 O_2
 O_1
 O_2
 O_1
 O_2

RN 4334-23-0 CAPLUS

CN Pyridine, 4,4'-s-triazole-3,5-diyldi-, dihydrochloride (8CI) (CA INDEX NAME)

●2 HCl

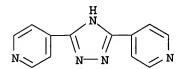
RN 4334-24-1 CAPLUS

CN Pyridine, 4,4'-s-triazole-3,5-diyldi-, dinitrate (8CI) (CA INDEX NAME)

CM 1

CRN 7697-37-2 CMF H N O3

CRN 4329-78-6 CMF C12 H9 N5



ANSWER 48 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1963:14876 CAPLUS

DOCUMENT NUMBER: 58:14876 58:2449a ORIGINAL REFERENCE NO.:

TITLE: Synthesis of 3,5-diaryl-1,2,4-triazole

AUTHOR (S): Kubota, Seiju; Ohtsuka, Michiko

Univ. Tokushima CORPORATE SOURCE:

Tokushima Daigaku Yakugakubu Kenkyu Nenpo (1960), 9, SOURCE:

15-18

CODEN: TDYKA8; ISSN: 0371-6139

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

RCONHNHCOR' and NH4Cl (2 equivs.) heated 3 hrs. at 260-70° gave the corresponding 3,5-(R, R' substituted)-1,2,4-triazole (R, R', and % yield given): Ph, Ph, 68; PhCH2, PhCH2, 11; Ph, 4-MeC6H4, 10; 4-pyridyl, 4-pyridyl, 45; Ph, 4-pyridyl, 33; Ph, 2-pyridyl, 5; 2-pyridyl, 2-pyridyl,

5. The use of urea or benzenesulfonamide instead of NH4Cl decreased the yield. 4329-78-6P, Pyridine, 4,4'-s-triazole-3,5-diyldi-IT

RL: PREP (Preparation) (preparation of)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

ANSWER 49 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

1960:129096 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 54:129096

ORIGINAL REFERENCE NO.: 54:24790h-i,24791a-d

TITLE: Preparation of 1,2,4,5-tetrazines from pyridine and

methylenedioxybenzene

AUTHOR(S): Dallacker, F.

CORPORATE SOURCE: Tech. Hochschule, Aachen, Germany

SOURCE: Monatshefte fuer Chemie (1960), 91, 294-304

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

Pyridine-2-carbonitrile, the 3- and 4-isomer, and 3,4methylenedioxybenzonitrile were treated with N2H4.H2O (I) to give the corresponding 1,2-dihydro-1,2,4,5-tetrazine (II), which was oxidized with HNO3 to the 1,2,4,5-tetrazine (III), or the pyridine compds. were rearranged with HCl to a 3,5-disubstituted-4-amino-1,2,4-triazole (IV). A

mixture of 46.8 g. pyridinecarbonitrile and 200 ml. of 80% I was heated on a steam-bath and a small amount of Raney Ni added. Heating was continued until a solid formed, and after 10 min., 500 ml. ice water was added and 3,6-dipyridyl derivative of II separated and some IV remained in the filtrate. Thus prepared were II (pyridine isomer, m.p., crystallization solvent, % yield, and color given): 2, 194.2°, iso-PrOH, 85.5, yellow; 3, 235.2°, pyridine, 46.2, orange; 4, 275.5°, HOAc-H2O, 72.4, orange. Similarly, 49 g. 3,4-methylenedioxybenzonitrile, 150 ml. 80% I, and 23 g.

H2NNH2.HCl gave 3,6-bis(3,4-methylenedioxyphenyl) derivative of II, m. 242.5° (HOAc), 51.8% yield, yellow. A solution of 2 g. 3,6-disubstituted derivative of II in 100 ml. HOAc was treated during 10 min. with 10 ml. 5N HNO3 and with cooling or by adding 1 ml. HNO3 gave the salt

of III which was crystallized from pyridine (V) to give the base. Thus prepared

were III (3,6-substitution, m.p., crystallization solvent, % yield, and color given): 2-pyridyl, 224.5°, iso-PrOH, 81.5, red; 3-pyridyl, 198.2°, EtOH, 80.4, blue-red; 4-pyridyl, 256.8°, HCONMe2, 89.4, violet; 3,4-methylenedioxyphenyl, 270.5°, HCONMe2, 98.5, red; 2-thienyl, 226.5°, EtOH, 40.2, red. A mixture of 10 g. 3,6-dipyridyl derivative of II and 200 ml. N HCl was heated 12-15 min. and the clear solution made alkaline with N NH3 to give a crude product. This was heated for 5-6 hrs. with 50 g. Raney Ni in 3 l. iso-PrOH, filtered hot, and IV crystallized from the filtrate. Thus prepared were the following IV (3,5-substitution, m.p. crystallization solvent, and % yield given): 2-pyridyl, 184.8°, iso-PrOH, 45.2; 3-pyridyl, 275.5°, iso-PrOH, 63.2; 4-pyridyl, 328.6° (decomposition), H2O, 58.4. To a solution of 8 g. 3,6-bis(3,4-methylenedioxyphenyl) derivative of II in 300 ml. boiling HOAc was added 100 ml. N HCl. After heating the mass 10 min., it was concentrated in vacuo and 3,5-bis(3,4-methylenedioxyphenyl)-1,2,4-oxadiazole separated, m. 242.8° (HCONMe2), in 15% yield. Concentration of the filtrate gave 1,2-bis(3,4-methylenedioxybenzoyl)hydrazine, m. 234.5° (HOAc-H2O), in 24% yield. Infrared data supported the structures given.

38634-05-8P, 4H-1,2,4-Triazole, 4-amino-3,5-di-4-pyridyl-IT RL: PREP (Preparation)

(preparation of)

RN 38634-05-8 CAPLUS

CN4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)

ANSWER 50 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1959:106842 CAPLUS

DOCUMENT NUMBER: 53:106842 ORIGINAL REFERENCE NO.: 53:19169c-d

Search for tuberculostatics. VI. Some new derivatives TITLE:

of isonicotinic acid-hydrazide

AUTHOR (S): Zsolnai, Tibor

CORPORATE SOURCE: Univ. Debrecen, Hung.

SOURCE: Zentralblatt fuer Bakteriologie, Parasitenkunde,

Infektionskrankheiten und Hygiene, Abteilung 1:

Medizinisch-Hygienische Bakteriologie, Virusforschung und Parasitologie, Originale (1959), 175, 269-81

CODEN: ZBPHA6; ISSN: 0372-8110

DOCUMENT TYPE: Journal LANGUAGE: German

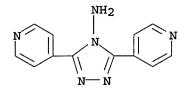
GI For diagram(s), see printed CA Issue.

AB cf. C.A. 53, 17336c. Some derivs. of isonicotinic acid hydrazide were tested and their tuberculostatic activity tested in vitro. Only those compds. which contained the C:C.N:C.C:CCONHN group were tuberculostatic. 34 references.

IT 38634-05-8, Pyridine, 4,4'-(4-amino-4H-1,2,4-triazole-3,5-diyl)di-(tuberculostatic action of)

RN 38634-05-8 CAPLUS

'CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)



L4 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1958:113705 CAPLUS

DOCUMENT NUMBER: 52:113705 ORIGINAL REFERENCE NO.: 52:20151g-h

TITLE: The product from condensation of isonicotinic acid

with hydrazine hydrate

AUTHOR(S): Yashunskii, V. G.; Pavlov, L. N.; Ermolaeva, V. G.;

Schukina, M. N.

SOURCE: Meditsinskaya Promyshlennost SSSR (1957), 11(No. 12),

38-40

CODEN: MPSSA9; ISSN: 0369-1586

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB The by-product formed during condensation of isonicotinic acid and hydrazine hydrate was identified tentatively as 2,5-di(4-pyridyl)-1-amino-1,3,4-triazole. The aminotriazole cycle possesses great stability and the amino group can be split off. However, it cannot form salts. It melts at 330-33° with decomposition Picric acid and HCl yield dipicrate and dihydrochloride. Heating with KMnO4 or HNO3 yields 2,5-di(4-pyridyl)-1,3,4-triazole. Heating with benzaldehyde yields a compound having the formula C19H14N6.H2O.

IT 38634-05-8, Pyridine, 4,4'-(4-amino-4H-1,2,4-triazole-3,5-diyl)di-(and derivs.)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)

IT 4329-78-6P, Pyridine, 4,4'-s-triazole-3,5-diyldi-111274-04-5P, Pyridine, 4,4'-(4-benzylideneamino-4H-1,2,4-triazole-

3,5-diyl)di-

RL: PREP (Preparation)

(preparation of)

RN 4329-78-6 CAPLUS

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

RN 111274-04-5 CAPLUS

CN Pyridine, 4,4'-(4-benzylideneamino-4H-1,2,4-triazole-3,5-diyl)di- (6CI) (CA INDEX NAME)

4 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1958:35257 CAPLUS

DOCUMENT NUMBER: 52:35257
ORIGINAL REFERENCE NO.: 52:6345f-q

TITLE: 2,5-Di(4-pyridyl)-1-amino-1,3,4-triazole and its

derivatives

AUTHOR(S): Yashunskii, V. G.; Pavlov, L. N.; Ermolalva, V. G.;

Shchukina, M. N.

SOURCE: Khimicheskaya Nauka i Promyshlennost (1957), 2, 658

CODEN: KHNPAX; ISSN: 0368-5586

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB In the condensation of isonicotinic acid with hydrazine hydrate besides the by-product 1,2-diisonicotinoyl a new product was found which is probably 2,5-di(4-pyridyl)-1-amino-1,3,4-triazole (I), stable in boiling HCl. K2MnO4 and concentrated HNO3 reacted with I to give 2,5-di(4-pyridyl)-1,3,4-triazole (II), m. 286-9°. Its di-HCl salt (m. 300-2°) and its dipicrate (m. 257-9°) were prepared Boiling I with PhCHO at 150-5° gave the benzaldazine derivs. of II (m. 197-200°) and of 2,4-di(4-pyridyl)triazole, m. 286-9°.

IT 38634-05-8, Pyridine, 4,4'-(4-amino-4H-1,2,4-triazole-3,5-diyl)di-(and derivs.)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)

IT 4329-78-6P, Pyridine, 4,4'-s-triazole-3,5-diyldi-111274-04-5P, Pyridine, 4,4'-(4-benzylideneamino-4H-1,2,4-triazole-

3,5-diyl)di-

RL: PREP (Preparation)

(preparation of)

RN 4329-78-6 CAPLUS

Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

RN111274-04-5 CAPLUS

CN Pyridine, 4,4'-(4-benzylideneamino-4H-1,2,4-triazole-3,5-diyl)di- (6CI) (CA INDEX NAME)

ANSWER 53 OF 53 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1957:9360 CAPLUS

DOCUMENT NUMBER: 51:9360

ORIGINAL REFERENCE NO.: 51:1957e-i,1958a-e

TITLE: Congeners of pyridine-4-carboxyhydrazide. I.

Derivatives of 4-cyanopyridine and 2-cyanothiazole

AUTHOR (S): Libman, D. D.; Slack, R.

CORPORATE SOURCE: May & Baker Ltd., Dagenham, UK

SOURCE: Journal of the Chemical Society (1956) 2253-7

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal LANGUAGE: Unavailable OTHER SOURCE(S): CASREACT 51:9360

4-Cyanopyridine (I) was converted into pyridine-4-carboxamidrazone (II), and several dipyridyl heterocyclic secondary products were isolated. 2-Cyanothiazole (III) and some derivs. were also prepared I (150 g.) in CHCl3 and EtOH treated with anhydrous HCl (IV) at 0° until a semi-solid upper layer separated, the vessel kept sealed 24 hrs. at 0°, the contents treated at 0° with 50% NaOH, the crude imidoate added to 372 ml. EtOH, 83 ml. 100% N2H4.H2O (IVa), 105 ml. H2O, and 114 ml. concentrated HCl at 5°, and the mixture kept at 0° for 2 hrs. gave 17 g. II.HCl as prisms, m. 280° (decomposition). The original filtrate heated 3 hrs. at 100° yielded 60 g. 1,2-dihydro-3,6-di(4-pyridyl)-1,2,4,5-tetrazine (V) as orange needles, m. 275°. Yields of II of 28% were obtained in smaller-scale expts., but with a corresponding lower yield of V. Crude imidoate base (from 40 g. I) treated at 0° with a neutral solution of 16.5 ml. IVa, EtOH, H2O, and 33 ml. concentrated HCl for 1

hr. gave yellow plates of the diimine, m. above 280° (decomposition). At 100° the plates were converted into 5.2 g. 1,2-di(pyridine-4carboxyimidoyl)hydrazine as an amorphous solid of the same m.p. The original filtrate heated 3 hrs. at 100° gave 15.4 g. of V and 1 g. 3,5-di(4-pyridyl)-1,2,4-triazole (VI), m. 283° (from EtOH). VI was also prepared by dissolving the crude hydrochloride of the above diimine in hot H2O and refluxing. The bismethotoluene-p-sulfonate formed prisms, m. 188° (from MeOH-Me2CO). In the following methods crude VI was purified by dissolution in cold 2N NaOH and repptn. with 2N AcOH followed by crystallization from alc. Pyridine-4-carboxyhydrazide heated with an equimolar

amount of pyridine-4-carboxamide at 220-40° for 1 hr., or 0.5 hr. at 140-50° with pyridine-4-thiocarboxamide (VII) gave VI in yields of 5% and 27%, resp. V (4.76 g.) refluxed 6 hrs. in EtOH-KOH gave 1.2 g. VI. II.HCl (4 g.) heated 45 min. at 130° in a sealed tube with H2O gave 0.4 g. VI and 0.2 g. V. II (18.2 g.) in 2N AcOH treated 2 hrs. at 0° with 7.5 g. NaNO2 in H2O yielded 10.5 g. 5-(4-pyridyl)-1,2,3,4tetrazole, prisms, m. 262-3° (decomposition). V (32 g.) in hot 50% AcOH poured into 6.5 l. cold solvent and treated below 15° with 9.4 q. NaNO2 in a little H2O gave 21 g. 3,6-di(4-pyridyl)-1,2,4,5-tetrazine (VIII), m. 258° (decomposition); bismetho(methyl sulfate) (95% yield), m. 200° (decomposition). VIII refluxed 5 min. with 2N Na2CO3 gave 56% RCH:NNHCOR(R = 4-pyridyl) (IX), needles, m. 230° (from H2O). Pyridine-4-carboxyhydrazide and 4-formylpyridine refluxed 1 hr. gave IX as prisms, m. 232° (from MeNO2). V (37 g.) suspended in 370 ml. 2N HCl and refluxed 8-9 min. gave 22 g. 4-amino-3,5-di(4-pyridyl)4,1,2triazole (X) dihydrochloride as prisms, m. 312° (from 4N HCl), converted by 2N NH3 into free X, m. 335-40° (decomposition). filtrate yielded 15 g. 1,2-di(pyridine-4-carbonyl)hydrazine (XI) as needles, m. 250°. XI (108 g.) added portionwise below 35°. to 270 ml. concentrated H2SO4, heated 10 min. at 100°, and the cooled solution neutralized with NH4OH gave 32 g. 2,5-di(4-pyridyl)-1,3,4-oxadiazole as needles, m. 185° (from H2O or MeOH); bismethiodide (57% yield), orange needles, m. 278°. VII (330 g.), 620 ml. EtOH, and 130 ml. IVa warmed at 40°, after the evolution of H2S had subsided the mixture refluxed 1 hr., and the product purified gave an acetate which dissociated at 100° to give 140 g. V. The AcOH filtrate concentrated to dryness and the residue extracted with C5H5N gave 30 g. 2,5-di(4-pyridyl)1,3,4thiadiazole as plates, m. 243°. The residue from 2N HCl gave 35 g. X dihydrochloride. The original aqueous extract gave a residue which when fractionally crystallized gave small amts. of plates, m. 227°, and needles, m. 285° (from aqueous alc.). I (5 g.) in 25 ml. PhCH2SH saturated in the cold with IV and kept at room temperature for 5 days and the crude thioester hydrochloride added portionwise to 5 ml. IVa in EtOH, and the solution made neutral, left 1 week, and the precipitated solid collected

gave

CN

1.5 g. V, a little of VIII, and (PHCH2)2S, m. 69-70°. Basification of the filtrate gave 1.2 g. X. An intimate mixture of 64 g. thiazole-2-carboxamide mixed with 10 ml. 100% IVa at 0° yielded 8 g. thiazole-2-carboxamidrazone as needles, m. 106° (from ligroine). IVa (20 ml.) and 20 g. III first cooled and then heated 3 hrs. yielded 7 g. 1,2(or 1,4)-dihydro-3,6-di(2-thiazolyl)-1,2,4,5-tetrazine, orange needles, m. 209° (decomposition) (from aqueous C5H5N). III (30 g.) in EtOH treated with 240 ml. saturated EtOH-NH3, then saturated at 0° with H2S, left 2 hrs. and purified gave 24 g. thiazole-2-thiocarboxamide as plates, m. 176° (from H2O).

IT 4329-78-6P, Pyridine, 4,4'-s-triazole-3,5-diyldi38634-05-8P, Pyridine, 4,4'-(4-amino-4H-1,2,4-triazole-3,5-diyl)di108564-98-3P, Pyridine, 4,4'-(4-amino-4H-1,2,4-triazole-3,5-diyl)di-, dihydrochloride 124359-89-3P, Pyridine,
4,4'-s-triazole-3,5-diyldi-, dimetho-p-toluenesulfonate
RL: PREP (Preparation)
(preparation of)

RN 4329-78-6 CAPLUS

Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

RN 38634-05-8 CAPLUS

CN 4H-1,2,4-Triazol-4-amine, 3,5-di-4-pyridinyl- (9CI) (CA INDEX NAME)

RN 108564-98-3 CAPLUS

CN Pyridine, 4,4'-(4-amino-4H-1,2,4-triazole-3,5-diyl)di-, dihydrochloride (6CI) (CA INDEX NAME)

●2 HCl

RN 124359-89-3 CAPLUS

CN Pyridine, 4,4'-s-triazole-3,5-diyldi-, dimetho-p-toluenesulfonate (6CI) (CA INDEX NAME)

CM 1

CRN 4329-78-6 CMF C12 H9 N5

. CM 2

CRN 80-48-8 CMF C8 H10 O3 S

=> => file uspatall

FILE 'USPATFULL' ENTERED AT 15:49:54 ON 18 JAN 2007

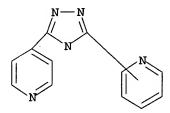
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FILE 'USPAT2' ENTERED AT 15:49:54 ON 18 JAN 2007

CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

=> d que

L1 STR



Structure attributes must be viewed using STN Express query preparation.

L3 81 SEA FILE=REGISTRY SSS FUL L1

L5 13 SEA L3

=> d 15 1-13 ibib abs hitstr

L5 ANSWER 1 OF 13 USPATFULL on STN

ACCESSION NUMBER: 2006:222524 USPATFULL

TITLE: Process for producing 1,2,4-triazole compound and

intermediate therefor

INVENTOR(S): Nakamura, Hiroshi, Saitama-shi, JAPAN

Uda, Junichiro, Saitama-shi, JAPAN Ohno, Atsushi, Saitama-shi, JAPAN Sato, Takahiro, Saitama-shi, JAPAN

PATENT ASSIGNEE(S): FUJIYAKUHIN CO., LTD., Saitama, JAPAN (non-U.S.

corporation)

NUMBER KIND DATE -----PATENT INFORMATION: US 2006189811 **A**1 20060824 US 2004-565678 APPLICATION INFO.: A1 20040723 (10) WO 2004-JP10456 20040723 20060124 PCT 371 date

DOCUMENT TYPE: Utility FILE SEGMENT: APPLICATION

LEGAL REPRESENTATIVE: OBLON, SPIVAK, MCCLELLAND, MAIER & NEUSTADT, P.C., 1940

DUKE STREET, ALEXANDRIA, VA, 22314, US

NUMBER OF CLAIMS: 10
EXEMPLARY CLAIM: 1
LINE COUNT: 1031

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

Provided is a process for producing 1,2,4-triazole compound (5), or a salt or hydrate thereof which comprises reacting compound (1) with Rc-X (2) to give compound (3), reacting compound (3) with a nitrilization agent to give compound (4), and then removing the group Rc, as shown by the reaction scheme: ##STR1## (Wherein Ra, Rb and Rd represent a group, Rc represents a group which can be removed by an acid) A 1,2,4-triazole compound (5) having an optionally substituted 2-cyanopyridin-4-yl group at 3-position and an optionally substituted aromatic group at 5-position which inhibits a xanthine oxidase and is

useful for treatment of gout and hyperuricemia can be obtained from compound (1) in a high yield without requiring isolation of reaction products in the course of reactions.

'CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 36770-53-3P 837371-71-8P 837371-86-5P

837371-87-6P 837371-88-7P

(intermediate; preparation of 1,2,4-triazole derivs.)

RN 36770-53-3 USPATFULL

CN Pyridine, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 1-oxide (9CI) (CA INDEX NAME)

RN 837371-71-8 USPATFULL

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 577778-58-6 CMF C13 H8 N6

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 837371-86-5 USPATFULL

CN Pyridine, 2-methyl-4-[5-(1-oxido-4-pyridinyl)-1H-1,2,4-triazol-3-yl](9CI) (CA INDEX NAME)

RN 837371-87-6 USPATFULL

CN Pyridine, 2-chloro-4-[5-(1-oxido-4-pyridinyl)-1H-1,2,4-triazol-3-yl](9CI) (CA INDEX NAME)

RN 837371-88-7 USPATFULL

CN Pyridine, 4-[5-(1-oxido-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-2-phenyl-(9CI) (CA INDEX NAME)

IT 577778-58-6P 577778-84-8P 837371-75-2P

837371-76-3P 837371-77-4P 837371-81-0P

837371-85-4P

(preparation of 1,2,4-triazole derivs.)

RN 577778-58-6 USPATFULL

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 577778-84-8 USPATFULL

CN 2-Pyridinecarbonitrile, 4-[5-(2-chloro-4-pyridinyl)-1H-1,2,4-triazol-3-yl](9CI) (CA INDEX NAME)

RN 837371-75-2 USPATFULL

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 837371-76-3 USPATFULL
CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-,
sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 577778-58-6 CMF C13 H8 N6

CM 2

CRN 7664-93-9 CMF H2 O4 S

RN 837371-77-4 USPATFULL CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, methanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 577778-58-6 CMF C13 H8 N6

CRN 75-75-2 CMF C H4 O3 S

RN 837371-81-0 USPATFULL

CN 2-Pyridinecarbonitrile, 4-[5-(2-methyl-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 577778-70-2 CMF C14 H10 N6

$$\begin{array}{c|c} N & H & N \\ \hline N & N & CN \\ \end{array}$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 837371-85-4 USPATFULL

CN 2-Pyridinecarbonitrile, 4-[5-(2-phenyl-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 577778-85-9 CMF C19 H12 N6

CM 2

CRN 104-15-4

CMF C7 H8 O3 S

L5 ANSWER 2 OF 13 USPATFULL on STN

ACCESSION NUMBER: 2005:5069 USPATFULL

TITLE: Novel 1 2 4-triazole compound

INVENTOR(S): Nakamura, Hiroshi, Nagareyama-shi, JAPAN

Kaneda, Soichi, Shiki-shi, JAPAN Sato, Takahiro, Kita-ku, JAPAN

Ashizawa, Naoki, Kamifukuoka-shi, JAPAN Matsumoto, Koji, Saitama-shi, JAPAN Iwanaga, Takashi, Kazo-shi, JAPAN Inoue, Tsutomu, Funabashi-shi, JAPAN

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2005004175	A1	20050106	
	US 7074816	B2	20060711	
APPLICATION INFO.:	US 2004-495322	A1	20040511	(10)
	WO 2002-JP12662		20021203	

NUMBER	DATE
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PRIORITY INFORMATION: JP 2002-17825 20020128

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION

LEGAL REPRESENTATIVE: PRICE HENEVELD COOPER DEWITT & LITTON, LLP, 695

KENMOOR, S.E., P O BOX 2567, GRAND RAPIDS, MI, 49501

NUMBER OF CLAIMS: 9
EXEMPLARY CLAIM: 1
LINE COUNT: 787

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A novel 1,2,4-triazole compound which is useful as a therapeutic agent for hyperuricemia and gout due to hyperuricemia is provided. A compound is represented by the following general formula (1): ##STR1##

wherein R.sub.2 represents an unsubstituted or substituted pyridyl group, R.sub.1 represents a similar pyridyl group, a pyridine-N-oxide group corresponding to these pyridyl groups, or a phenyl group, and R.sub.3 represents hydrogen or a lower alkyl group substituted with pivaloyloxy group and R.sub.3 bonds to a nitrogen atom in the ring. A process for production of a compound by reacting a nitrile and a hydrazide, and a therapeutic agent, particularly a xanthine oxidase inhibitor are also provided.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 577778-58-6P 577778-70-2P 577778-74-6P

577778-82-6P 577778-84-8P 577778-85-9P

(preparation of 1,2,4-triazole derivs. for treatment of hyperuricemia)

RN 577778-58-6 USPATFULL

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 577778-70-2 USPATFULL CN 2-Pyridinecarbonitrile, 4-[5-(2-methyl-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & H & N \\ \hline N & N & CN \\ \end{array}$$

RN 577778-74-6 USPATFULL CN Pyridine, 2-chloro-4-[5-(2-methyl-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

$$N$$
 N
 N
 N
 N
 M
 M

RN 577778-82-6 USPATFULL CN 2-Pyridinecarbonitrile, 4-[5-(1-oxido-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

RN 577778-84-8 USPATFULL CN 2-Pyridinecarbonitrile, 4-[5-(2-chloro-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

RN 577778-85-9 USPATFULL CN 2-Pyridinecarbonitrile, 4-[5-(2-phenyl-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

IT 577778-88-2P

(preparation of 1,2,4-triazole derivs. for treatment of hyperuricemia)

RN 577778-88-2 USPATFULL

CM 1

CRN 577778-58-6 CMF C13 H8 N6

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L5 ANSWER 3 OF 13 USPATFULL on STN

ACCESSION NUMBER:

PATENT ASSIGNEE(S):

2002:160747 USPATFULL

TITLE:

INVENTOR(S):

3-(substituted pyridyl)-1,2,4-triazole compounds Tisdell, Francis E., Carmel, IN, United States Johnson, Peter L., Indianapolis, IN, United States Pechacek, James T., Indianapolis, IN, United States

Bis, Scott J., Carmel, IN, United States

Hegde, Vidyadhar B., Carmel, IN, United States

Schoonover, Jr., Joe R., Brownsburg, IN, United States Dintenfass, Leonard P., Indianapolis, IN, United States

Gifford, James M., Lebanon, IN, United States
DeVries, Donald H., Fishers, IN, United States
Martin, Timothy P., Indianapolis, IN, United States
Pine Porty V. Sir Project M. United States

Ripa, Perry V., Sun Prairie, WI, United States
Dow AgroSciences LLC, Indianapolis, IN, United States

(U.S. corporation)

NUMBER	KIND	DATE	
US 6413992 US 1999-425091	B1	20020702	(9)

NUMBER DATE

PRIORITY INFORMATION: US 1998-105356P 19981023 (60)

DOCUMENT TYPE: Utility FILE SEGMENT: GRANTED

PRIMARY EXAMINER: Morris, Patricia L.

LEGAL REPRESENTATIVE: Stuart, Donald R., Mixan, Craig E.

NUMBER OF CLAIMS: 9 EXEMPLARY CLAIM: 1

NUMBER OF DRAWINGS: 0 Drawing Figure(s); 0 Drawing Page(s)

LINE COUNT: 1129

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Compounds of the formula ##STR1##

wherein one of X and Y is lower alkyl, haloalkyl, lower alkenyl, lower alkynyl, or alkoxyalkyl; and the other of X and Y is optionally substituted phenyl, pyridyl, thienyl, cyclopropyl, or thiazolyl; and Z is subtituted pyridyl are useful as insecticides and acaricides. New synthetic procedures and intermediates for preparing the compounds, pesticide compositions containing the compounds, and methods of controlling insects and mites using the compounds are also provided.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 265985-45-3P

(preparation of pyridyl-1,2,4-triazoles as acaricides and insecticides) RN 265985-45-3 USPATFULL

CN Pyridine, 3,5-dichloro-4-[5-[6-(methylthio)-3-pyridinyl]-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

L5 ANSWER 4 OF 13 USPATFULL on STN

ACCESSION NUMBER: 78:49009 USPATFULL

TITLE: Anti-hyperuricemia composition

INVENTOR(S): Novello, Frederick C., Berwyn, PA, United States

Baldwin, John J., Lansdale, PA, United States

PATENT ASSIGNEE(S): Merck & Co., Inc., Rahway, NJ, United States (U.S.

corporation)

NUMBER KIND DATE

PATENT INFORMATION: US 4111944 19780905 APPLICATION INFO.: US 1977-808575 19770621 (5)

RELATED APPLN. INFO.: Continuation of Ser. No. US 1976-742945, filed on 18

Nov 1976, now abandoned which is a continuation of Ser. No. US 1975-547848, filed on 6 Feb 1975, now abandoned which is a continuation of Ser. No. US 1973-361915, filed on 21 May 1973, now patented, Pat. No. US 3892762

which is a continuation-in-part of Ser. No. US 1970-75784, filed on 25 Sep 1970, now abandoned

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Randolph, John D.

LEGAL REPRESENTATIVE: Sudol, Jr., Michael C., Szura, Daniel T.

NUMBER OF CLAIMS:

3

EXEMPLARY CLAIM:

1

LINE COUNT:

494

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compos contai

Compositions useful in the treatment of gout and hyperuricemia and containing a substituted 1,2,4-triazole as the active ingredient are provided, the triazoles being substituted at the 5 position with a pyridyl radical and at the 3 position with a phenyl or a pyridyl radical. Methods of preparing these substituted triazoles are described. Certain of the compounds are novel.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 36770-45-3P 36770-46-4P 36770-47-5P

36770-48-6P 36770-50-0P 36770-51-1P

36770-53-3P

(preparation of)

RN 36770-45-3 USPATFULL

CN Pyridine, 2-methyl-4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-46-4 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & H & N \\ \hline N & N & Me \end{array}$$

RN 36770-47-5 USPATFULL

CN Pyridine, 2,6-dimethyl-4-[5-(4-pyridinyl-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-48-6 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2,6-dimethyl- (9CI) (CA INDEX NAME)

RN 36770-50-0 USPATFULL

CN Pyridine, 2-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-51-1 USPATFULL

CN Pyridine, 3-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-53-3 USPATFULL

CN Pyridine, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 1-oxide (9CI) (CA INDEX NAME)

L5 ANSWER 5 OF 13 USPATFULL on STN

ACCESSION NUMBER:

77:49489 USPATFULL

TITLE: INVENTOR(S): 1,3,5-Trisubstituted-1,2,4-triazole compounds
Baldwin, John J., Lansdale, PA, United States
Nevello Frederick C. Porver PA United States

PATENT ASSIGNEE(S):

Novello, Frederick C., Berwyn, PA, United States Merck & Co., Inc., Rahway, NJ, United States (U.S.

corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 4048183		19770913	
APPLICATION INFO.:	US 1976-672899		19760402	(5)

RELATED APPLN. INFO.:

Division of Ser. No. US 1975-599504, filed on 28 Jul 1975, now patented, Pat. No. US 3978054 which is a

division of Ser. No. US 1974-527992, filed on 29 Nov

1974, now patented, Pat. No. US 3928361 which is a division of Ser. No. US 1973-361914, filed on 21 May

1973, now patented, Pat. No. US 3882134

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Jaisle, Cecilia M. S.

LEGAL REPRESENTATIVE: Szura, Daniel T., Behan, J. Jerome

NUMBER OF CLAIMS: EXEMPLARY CLAIM: LINE COUNT: 152

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

Compounds useful in the treatment of asthma, the symptoms of allergy and in some instances in gout and hyperuricemia are described. The novel

compounds are 1-substituted-1,2,4-triazoles being additionally

substituted at the 3- and 5-positions with a pyridyl radical. Methods of preparing these tri-substituted triazoles are described.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 4329-78-6 36770-51-1

(reaction of, with organic halides)

RN4329-78-6 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

RN 36770-51-1 USPATFULL

CN Pyridine, 3-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

ANSWER 6 OF 13 USPATFULL on STN

ACCESSION NUMBER: 76:54567 USPATFULL

TITLE: 1,3,5-Trisubstituted-1,2,4-triazole compounds used as

bronchodilators

INVENTOR (S): Baldwin, John J., Lansdale, PA, United States

Novello, Frederick C., Berwyn, PA, United States

PATENT ASSIGNEE(S): Merck & Co., Inc., Rahway, NJ, United States (U.S.

corporation)

NUMBER	KIND	DATE
•		

PATENT INFORMATION: US 3984558 19761005 APPLICATION INFO.: US 1974-527994 19741129 (5)

RELATED APPLN. INFO.: Division of Ser. No. US 1973-361914, filed on 21 May

1973, now patented, Pat. No. US 3882134

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Schenkman, Leonard

LEGAL REPRESENTATIVE: Szura, Daniel T., Behan, J. J.

NUMBER OF CLAIMS: 12
EXEMPLARY CLAIM: 1
LINE COUNT: 150

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compounds useful in the treatment of asthma, the symptoms of allergy and in some instances in gout and hyperuricemia are described. The novel compounds are 1-substituted-1,2,4-triazoles being additionally substituted at the 3- and 5-positions with a pyridyl radical. Methods of preparing these tri-substituted triazoles are described.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 4329-78-6

(alkylation of)

RN 4329-78-6 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

L5 ANSWER 7 OF 13 USPATFULL on STN

ACCESSION NUMBER: 76:48023 USPATFULL

TITLE: 1,3,5-Trisubstituted-1,2,4-triazole compounds
INVENTOR(S): Baldwin, John J., Lansdale, PA, United States
Novello, Frederick C., Berwyn, PA, United States

PATENT ASSIGNEE(S): Merck & Co., Inc., Rahway, NJ, United States (U.S.

corporation)

RELATED APPLN. INFO.: Division of Ser. No. US 1974-527992, filed on 29 Nov

1974, now patented, Pat. No. US 3928361 which is a division of Ser. No. US 1973-361914, filed on 21 May

1973, now patented, Pat. No. US 3882134

(5)

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Trousof, Natalie ASSISTANT EXAMINER: Bond, Robert T.

LEGAL REPRESENTATIVE: Szura, Daniel T., Behan, J. Jerome

NUMBER OF CLAIMS: 4
EXEMPLARY CLAIM: 1
LINE COUNT: 161

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compounds useful in the treatment of asthma, the symptoms of allergy and in some instances in gout and hyperuricemia are described. The novel compounds are 1-substituted-1,2,4-triazoles being additionally substituted at the 3- and 5-positions with a pyridyl radical. Methods of preparing these tri-substituted triazoles are described.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 4329-78-6

(alkylation of)

RN 4329-78-6 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

L5 ANSWER 8 OF 13 USPATFULL on STN

ACCESSION NUMBER: 76:33638 USPATFULL

TITLE: Pyridyl containing 1-benzenesulfonyl triazoles

INVENTOR(S): Novello, Frederick C., Berwyn, PA, United States

Baldwin, John J., Lansdale, PA, United States

PATENT ASSIGNEE(S): Merck & Co., Inc., Rahway, NJ, United States (U.S.

corporation)

NUMBER KIND DATE

PATENT INFORMATION: US 3963731 19760615 APPLICATION INFO.: US 1975-547847 19750206 (5)

RELATED APPLN. INFO.: Division of Ser. No. US 1973-361915, filed on 21 May

1973, now patented, Pat. No. US 3892762 which is a continuation-in-part of Ser. No. US 1970-75784, filed

on 25 Sep 1970, now abandoned

DOCUMENT TYPE: Utility

FILE SEGMENT: Granted

PRIMARY EXAMINER: Jiles, Henry R. ASSISTANT EXAMINER: Ramsuer, R. W.

LEGAL REPRESENTATIVE: Szura, Daniel T., Behan, J. Jerome

NUMBER OF CLAIMS: 3
EXEMPLARY CLAIM: 1
LINE COUNT: 489

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

Compositions useful in the treatment of gout and hyperuricemia and containing a substituted 1,2,4-triazole as the active ingredient are provided, the triazoles being substituted at the 5 position with a pyridyl radical and at the 3 position with a phenyl or a pyridyl radical. Methods of preparing these substituted triazoles are described. Certain of the compounds are novel.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 4329-78-6

(acylation of)

RN 4329-78-6 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

IT 36770-45-3P 36770-46-4P 36770-47-5P

36770-48-6P 36770-50-0P 36770-53-3P

(preparation of)

RN 36770-45-3 USPATFULL

CN Pyridine, 2-methyl-4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-46-4 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} M & H & N \\ \hline M & N & M \end{array}$$

RN 36770-47-5 USPATFULL

CN Pyridine, 2,6-dimethyl-4-[5-(4-pyridinyl-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H \\ N \\ N \\ N \\ Me \end{array}$$

RN 36770-48-6 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2,6-dimethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{H} & \text{Me} \\ \hline & \text{N} & \text{N} & \text{Me} \\ \hline & \text{Me} & \text{Me} \\ \end{array}$$

RN 36770-50-0 USPATFULL

CN Pyridine, 2-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-53-3 USPATFULL

CN Pyridine, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 1-oxide (9CI) (CA INDEX NAME)

ANSWER 9 OF 13 USPATFULL on STN

ACCESSION NUMBER: 76:17380 USPATFULL

Anti-hyperuricemia composition TITLE:

Baldwin, John J., Lansdale, PA, United States INVENTOR (S):

Novello, Frederick C., Berwyn, PA, United States

Merck & Co., Inc., Rahway, NJ, United States (U.S. PATENT ASSIGNEE(S):

corporation)

KIND NUMBER DATE US 3947577 19760330

PATENT INFORMATION: US 1975-539488 APPLICATION INFO.: 19750108

RELATED APPLN. INFO.: Division of Ser. No. US 1973-361915, filed on 21 May

1973, now patented, Pat. No. US 3892762 which is a continuation-in-part of Ser. No. US 1970-75784, filed

(5)

on 25 Sep 1970, now abandoned

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Waddell, Frederick E.

LEGAL REPRESENTATIVE: Szura, Daniel T., Behan, J. Jerome

NUMBER OF CLAIMS: EXEMPLARY CLAIM: 1 LINE COUNT: 511

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

Compositions useful in the treatment of gout and hyperuricemia and containing a substituted 1,2,4-triazole as the active ingredient are provided, the triazoles being substituted at the 5 position with a pyridyl radical and at the 3 position with a phenyl or a pyridyl radical. Methods of preparing these substituted triazoles are described. Certain of the compounds are novel.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 36770-45-3 36770-47-5 36770-48-6

36770-50-0 36770-53-3

(antigout and antihyperuricemic agent)

RN 36770-45-3 USPATFULL

Pyridine, 2-methyl-4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA CN INDEX NAME)

36770-47-5 USPATFULL RN

Pyridine, 2,6-dimethyl-4-[5-(4-pyridinyl-1H-1,2,4-triazol-3-yl]- (9CI) CN

(CA INDEX NAME)

$$\begin{array}{c|c} H \\ N \\ N \\ N \\ Me \end{array}$$

RN 36770-48-6 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2,6-dimethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{H} & \text{Me} \\ \hline & \text{N} & \text{N} & \text{N} \\ \hline & \text{Me} & \text{Me} \\ \end{array}$$

RN 36770-50-0 USPATFULL

CN Pyridine, 2-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-53-3 USPATFULL

CN Pyridine, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 1-oxide (9CI) (CA INDEX NAME)

IT 36770-51-1

(in tablets, as antigout and antihyperuricemic agent)

RN 36770-51-1 USPATFULL

CN Pyridine, 3-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

IT 36770-46-4P

(preparation of)

RN 36770-46-4 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2-methyl- (9CI) (CA INDEX NAME)

IT 4329-78-6

(reaction of, with butyric anhydride)

RN 4329-78-6 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

L5 ANSWER 10 OF 13 USPATFULL on STN

ACCESSION NUMBER: 75:70247 USPATFULL

TITLE: 1-(Sulfamoylphenylalkyl)-3,5-dipyridyl-1,2,4 triazoles

INVENTOR(S): Baldwin, John J., Lansdale, PA, United States

Novello, Frederick C., Berwyn, PA, United States

PATENT ASSIGNEE(S): Merck & Co., Inc., Rahway, NJ, United States (U.S.

corporation)

NUMBER KIND DATE

PATENT INFORMATION: US 3928361 19751223 APPLICATION INFO.: US 1974-527992 19741129 (

RELATED APPLN. INFO.: Division of Ser. No. US 1973-361914, filed on 21 May

1973, now patented, Pat. No. US 3882134

DOCUMENT TYPE: Utility

FILE SEGMENT: Granted

PRIMARY EXAMINER: Jiles, Henry R. ASSISTANT EXAMINER: Ramsuer, R. W.

LEGAL REPRESENTATIVE: Szura, Daniel T., Behan, J. Jerome, Anderson, Jr.,

Rudolph J.

NUMBER OF CLAIMS: 3
EXEMPLARY CLAIM: 1
LINE COUNT: 129

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compounds useful in the treatment of asthma, the symptoms of allergy and in some instances in gout and hyperuricemia are described. The novel compounds are 1-substituted-1,2,4-triazoles being additionally

substituted at the 3- and 5-positions with a pyridyl radical. Methods of

preparing these tri-substituted triazoles are described.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 4329-78-6

(alkylation of)

RN 4329-78-6 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

L5 ANSWER 11 OF 13 USPATFULL on STN

ACCESSION NUMBER: 75:34468 USPATFULL

TITLE: Novel substituted 1,2,4-triazoles

INVENTOR(S): Baldwin, John J., Lansdale, PA, United States

Novello, Frederick C., Berwyn, PA, United States

PATENT ASSIGNEE(S): Merck & Co., Inc., Rahway, NJ, United States (U.S.

corporation)

NUMBER KIND DATE

PATENT INFORMATION: US 3892762 19750701

APPLICATION INFO.: US 1973-361915 19730521 (5)

RELATED APPLN. INFO.: Continuation-in-part of Ser. No. US 1970-75784, filed

on 25 Sep 1970, now abandoned

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Rotman, Alan L.

LEGAL REPRESENTATIVE: Szura, Daniel T., Behan, J. Jerome

NUMBER OF CLAIMS: 9
EXEMPLARY CLAIM: 1
LINE COUNT: 506

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compositions useful in the treatment of gout and hyperuricemia and containing a substituted 1,2,4-triazole as the active ingredient are provided, the triazoles being substituted at the 5 position with a pyridyl radical and at the 3 position with a phenyl or a pyridyl radical. Methods of preparing these substituted triazoles are described. Certain of the compounds are novel.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 36770-45-3P 36770-46-4P 36770-47-5P

36770-48-6P 36770-50-0P 36770-51-1P

36770-53-3P

(preparation of)

RN 36770-45-3 USPATFULL

CN Pyridine, 2-methyl-4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
N & N \\
N & N
\end{array}$$
Me

RN 36770-46-4 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2-methyl- (9CI) (CA INDEX

$$\stackrel{\mathsf{Me}}{\longrightarrow} \stackrel{\mathsf{N}}{\longrightarrow} \stackrel{\mathsf{N}}{$$

RN 36770-47-5 USPATFULL

CN Pyridine, 2,6-dimethyl-4-[5-(4-pyridinyl-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-48-6 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis[2,6-dimethyl-(9CI) (CA INDEX NAME)

RN 36770-50-0 USPATFULL

CN Pyridine, 2-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-51-1 USPATFULL

CN Pyridine, 3-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN 36770-53-3 USPATFULL

CN Pyridine, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, 1-oxide (9CI) (CA INDEX NAME)

L5 ANSWER 12 OF 13 USPATFULL on STN

ACCESSION NUMBER: 75:23843 USPATFULL

TITLE: 1-Substituted-3,5-dipyridyl-1,2,4-triazoles

INVENTOR(S): Baldwin, John J., Lansdale, PA, United States

Novello, Frederick C., Berwyn, PA, United States

PATENT ASSIGNEE(S): Merck & Co., Inc., Rahway, NJ, United States (U.S.

corporation)

NUMBER KIND DATE

PATENT INFORMATION: US 3882134 19750506

APPLICATION INFO.: US 1973-361914 19730521 (5)

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Rotman, Alan L.

LEGAL REPRESENTATIVE: Behan, J. Jerome, Szura, Daniel T.

NUMBER OF CLAIMS: 10 EXEMPLARY CLAIM: 1 LINE COUNT: 142

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compounds useful in the treatment of asthma, the symptoms of allergy and in some instances in gout and hyperuricemia are described. The novel

in some instances in gout and hyperuricemia are described. The novel

compounds are 1-substituted-1,2,4-triazoles being additionally

substituted at the 3- and 5-positions with a pyridyl radical. Methods of

preparing these tri-substituted triazoles are described.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 4329-78-6 36770-51-1

(reaction of, with organic halides)

RN 4329-78-6 USPATFULL

CN Pyridine, 4,4'-(1H-1,2,4-triazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)

RN 36770-51-1 USPATFULL

CN Pyridine, 3-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

ANSWER 13 OF 13 USPAT2 on STN

ACCESSION NUMBER: 2005:5069 USPAT2

TITLE:

1 2 4-triazole compound

INVENTOR(S):

Nakamura, Hiroshi, Nagareyama, JAPAN

Kaneda, Soichi, Shiki, JAPAN Sato, Takahiro, Kita-ku, JAPAN Ashizawa, Naoki, Kamifukuoka, JAPAN Matsumoto, Koji, Saitama, JAPAN Iwanaga, Takashi, Kazo, JAPAN Inoue, Tsutomu, Funabashi, JAPAN

PATENT ASSIGNEE(S):

Fuji Yakuhin Co., Ltd., Saitama, JAPAN (non-U.S.

corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 7074816 WO 2003064410	B2	20060711	
APPLICATION INFO.:	US 2002-495322 WO 2002-JP12662		20021203 20021203 20040511	(10) PCT 371 date

NUMBER DATE

PRIORITY INFORMATION:

JP 2002-17825 20020128

DOCUMENT TYPE:

Utility

FILE SEGMENT:

GRANTED

PRIMARY EXAMINER:

Saeed, Kamal A.

ASSISTANT EXAMINER:

Chung, Susannah L.

LEGAL REPRESENTATIVE:

Price, Heneveld, Cooper, DeWitt & Litton, LLP

NUMBER OF CLAIMS: EXEMPLARY CLAIM:

1

LINE COUNT:

771

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

A novel 1,2,4-triazole compound which is useful as a therapeutic agent for hyperuricemia and gout due to hyperuricemia is provided. A compound is represented by the following general formula (1):

wherein R.sub.2 represents an unsubstituted or substituted pyridyl group, R.sub.1 represents a similar pyridyl group, a pyridine-N-oxide group corresponding to these pyridyl groups, or a phenyl group, and R.sub.3 represents hydrogen or a lower alkyl group substituted with pivaloyloxy group and R.sub.3 bonds to a nitrogen atom in the ring. A process for production of a compound by reacting a nitrile and a hydrazide, and a therapeutic agent, particularly a xanthine oxidase inhibitor are also provided.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

577778-58-6P 577778-70-2P 577778-74-6P

577778-82-6P 577778-84-8P 577778-85-9P

(preparation of 1,2,4-triazole derivs. for treatment of hyperuricemia)

RN 577778-58-6 USPAT2

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

RN577778-70-2 USPAT2

CN2-Pyridinecarbonitrile, 4-[5-(2-methyl-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

577778-74-6 USPAT2 RN

CNPyridine, 2-chloro-4-[5-(2-methyl-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & H & N \\ N & N & Me \end{array}$$

RN 577778-82-6 USPAT2

CN2-Pyridinecarbonitrile, 4-[5-(1-oxido-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

RN577778-84-8 USPAT2

CN2-Pyridinecarbonitrile, 4-[5-(2-chloro-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

RN577778-85-9 USPAT2

CN2-Pyridinecarbonitrile, 4-[5-(2-phenyl-4-pyridinyl)-1H-1,2,4-triazol-3-yl]-(9CI) (CA INDEX NAME)

IT

(preparation of 1,2,4-triazole derivs. for treatment of hyperuricemia)

RN577778-88-2 USPAT2

CN 2-Pyridinecarbonitrile, 4-[5-(4-pyridinyl)-1H-1,2,4-triazol-3-yl]-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 577778-58-6 CMF C13 H8 N6

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

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